CENTER FOR ADVANCED PROCESS DECISION-MAKING

New Directions for Process Systems Engineering

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TABLE OF CONTENTS

GENERAL NEWS

Ignacio Grossmann will be taking over as Director of the CAPD on January 1, 2005 from **Larry Biegler,** who has served in this capacity since the designation of the CAPD as a CIT Center in 1999. The CAPD has had a strong history going back twenty years, and we are grateful for the interactions with our member companies. With this transition, we look forward to increasing these interactions in the future.

Larry Biegler has been selected winner of the 2005 Steve Fenves Award in Systems Engineering. He will receive the award at the College of Engineering Dinner on February 19, 2005. **Larry Biegler** and **Ignacio Grossmann** were elected Fellows of AIChE.

We are especially pleased to introduce two new member companies to the CAPD Center. **Cargill Corporation** recently joined with an interest in process synthesis and design for bioprocesses. In addition, **IBM Corporation** has started a research project with Ignacio Grossmann, Gerard Cornuejols and Larry Biegler on algorithms and applications for mixed integer nonlinear programming.

Pedro Castro from Instituto Superior Técnico, Lisbon, Portugal, and **Minhwan Park** from KAIST, Korea, have joined the group of Ignacio. Pedro will be working in the area of batch scheduling and Minhwan in the area of supply chain optimization. **Anna Bonfil** and **Gonzalo Guillen** from Polytechnic University of Barcelona (Puigjaner's group) visited Ignacio's group for 6 weeks to do research in batch scheduling. **Christos Maravelias**, a former Ph.D. student of Ignacio, has joined the Department of Chemical and Biological Engineering at the University of Wisconsin in Madison as an Assistant Professor**. Sarette Van den Heever**, also former Ph.D. student of Ignacio, received the W. David Smith Award for Best Graduate Student Paper from the CAST Division of AIChE. She received the award at the Annual AIChE Meeting in Austin.

We are pleased to welcome the following new graduate students into the CAPD group. **Brian Baumrucker** from the University of Kansas and **Victor Zavala** from the University of Iberoamericana have joined Larry Biegler's group. **Denny Jacob** from the University of Madras is working with Gary Powers. **Bora Terhan** from Bogazici University has joined Ignacio Grossmann's group. **Scott Turnberg** from the University of Massachusetts has joined Steinar Hauan's group and will be working on agent-based design of multiproduct reactive separation processes.

Congratulations to **Seth Knaebel**, who completed his MS degree in August with Larry Biegler. Seth's work dealt with the optimization of pressure swing adsorption systems for the separation of hydrogen and methane. He has taken a position with Adsorption Research, Inc. in Dublin, OH.

Congratulations to the following students who completed their Ph.D. qualifiers this fall: **Eduardo Dozal, Muge Erdirik, Xiang He, Ramkumar Karuppiah, Yoshi Kawajiri, and Israel Owusu.**

Proposal exams for **Juan Arrieta, Kendell Jillson, and Christy White** will be completed on December 15.

Ignacio Grossmann is organizing together with **Jaime Cerda** from INTEC, Argentina, and **Jose Pinto,** from Polytechnic University and University of Sao Paulo, the PanAmerican Study Institute on Process Systems Engineering that will take place in Iguazu Falls, Argentina, August 16-25, 2005. This is a workshop that is aimed at advanced graduate students. The major areas that will be covered are Optimization, Product and Process Design, Supply Chain Optimization and Process Control. It is expected that about 50 graduate students will participate (50% from US). Also, the different modules will be taught by leaders in the area, and the course material will be made available on the web. For more information see: http://cepac.cheme.cmu.edu/pasi.html

2005 ANNUAL REVIEW MEETING

The Annual Review Meeting will be held on March 7-8, 2005. The first day of the meeting will consist of overviews given by Larry, Ignacio, Erik, Steinar and Gary, followed by a discussion with industrial participants, and a poster session by the students. There will also be a dinner that evening at Le Mont Restaurant. The second day is devoted

to final year student presentations. Last year the feedback we received was extremely positive. If you have any additional thoughts or suggestions, please let us know.

2005 CAPD SHORT COURSE

Our short course, *Process Modeling and Optimization for Process Engineering* will be offered on May 18-24, 2005. In the past we were very pleased with the outcome of this course, as we have had attendees from around the world, both from industry and academia. For this year, the course has been extensively revised and includes the following modules:

a) Conceptual Design - taught on Wednesday and Thursday (May 18-19), with focus on support tools for design and information management, equation-based modeling and conceptual methods for process synthesis.

b) Optimization - taught on Friday and Saturday (May 20-21), with focus on modeling and algorithms for nonlinear programming and mixed integer programming including disjunctive programming and applications to process optimization.

c) Process Operations - taught on Monday and Tuesday (May 23-24), with focus on differential/algebraic models for real time optimization and parameter estimation, and on mixed-integer programming models for process scheduling and supply chain management.

The course included extensive workshops where participants obtained hands-on experience with various software packages. Course materials included extensive notes, the GAMS software, documentation and case study, and our textbook "Systematic Methods of Chemical Process Design." If you are interested in attending this course next summer, please contact Toni McIltrot at 412-268-3573, or e-mail: tm2l@andrew.cmu.edu.

WEBSITES/PROCESS SYSTEMS DIRECTORY

We are happy to report that the CAPD newsletter is distributed in electronic form. We would appreciate receiving feedback from our member companies of our CAPD website, **http://capd.cheme.cmu.edu.** This website provides a number of interesting items including information about individual groups, industrial success stories, software available from the group, etc. Other websites of interest are Ignacio's http://egon.cheme.cmu.edu, and Larry's http://dynopt.cheme.cmu.edu. Also, the department maintains the website of CEPAC (Chemical Engineering Pan American Collaboration), the organization that has been formed to promote collaboration between the US and Argentina, Brazil and Chile. You can find in **http://cepac.cheme.cmu.edu** a listing of all universities and researchers with links in the process systems area in the US, Argentina, Brazil, Canada and Chile. Mexico's will be added soon.

CAPD REPORT SERIES

Along with our web sites we have initiated a technical report series that covers the research output of our center. In addition to the reports that are regularly sent to our members, we are cataloging these reports on the web sites mentioned above. This allows us and other researchers to refer to these reports prior to their publication.

EXECUTIVE SUMMARY

Larry Biegler's Group

The past few months have seen a number of applications of dynamic optimization problems in the following areas:

Some time ago, we proved an equivalence of the optimality conditions for optimal control and our simultaneous nonlinear programming formulation based on orthogonal collocation on finite elements. **Shiva Kameswaran** has recently shown some very useful extensions to this work. He has shown an extension of the equivalence to Radau

collocation. Moreover, he has performed an analysis path constrained problems and demonstrated an interesting property that explains better performance of the simultaneous approach over conventional optimal control strategies. A paper that describes these concepts is listed below.

Nonlinear Model Predictive Control strategies are being explored with dynamic optimization tools centered on IPOPT. **Juan Arrieta** has developed NMPC strategies to determine near optimal trajectories for conflict resolution in aircraft and also in low-thrust vehicles. **Carl Laird** has expanded the source detection approach for municipal water networks to deal with moving spatial horizons in detecting contaminants in water network nodes. Publications that describe this work are listed below. Finally, **Victor Arrieta** has started a new project on NMPC for large-scale polymerization processes.

For periodic adsorption applications**, Daeho Ko** and **Seth Knaebel** have extended the optimization formulation of Dr. Ling Jiang (now at Air Products) to the gPROMS modeling environment. As noted in two papers below, both have done optimization on small pressure swing adsorption (PSA) cycles with binary separations. The optimization strategy appears to be fast and reliable and the resulting solutions show significant performance improvements over existing processes. In addition to this work, **Yoshi Kawajiri** is currently exploring similar optimization strategies for Simulated Moving Bed applications, the liquid-solid analog of PSA.

Enabling Software From Larry Biegler's Group

Highlights of **Larry Biegler's group** include further development of the interior point nonlinear programming algorithm, IPOPT, in a number of directions. **Andreas Waechter**, now at IBM, developed a novel and very efficient barrier (interior point) NLP method, based on many of our earlier SQP concepts. In the general purpose framework, it adopts a sparse decomposition of the KKT matrix, and has been tested on thousands of applications with up to a quarter of a million variables. It has also been used to solve problems that incorporate a number of specialized decomposition strategies and for a wide variety of applications with up to 2 million variables. IPOPT is available under an Open Source software license and the source code can be downloaded from http://www.coin-or.org/Ipopt/index.html.

Last summer, **Carl Laird** and **Andreas Waechter** have migrated the FORTRAN code for IPOPT into an object-oriented code written in C++. The resulting package leads to a much cleaner interface to modeling environments as well as a more efficient implementation of the algorithm. Finally, the object-oriented code allows for greater flexibility in adopting additional linear solvers and advanced decomposition strategies.

The IPOPT code has already been interfaced to a number of modeling systems including:

- **AIMMS** –This GAMS-like system has a number of extended features including a full graphical user interface for the development of specific user applications. Moreover, it provides exact first and second derivatives and exploits the full capabilities of IPOPT. **Yi-dong Lang** has nearly completed the interface to this system and is currently testing the interface. A similar interface to GAMS is also planned for January.
- **AMPL** – This GAMS-like system is the standard development platform in the Biegler group, has been available for the past two years and can be downloaded from the COIN-OR webpage. It has extensive features for linking to MATLAB and other environments in Unix and Windows. It also provides exact first and second derivatives and exploits the full capabilities of IPOPT.
- **MATLAB** – **Claas Michalik** and **Steinar Hauan** developed an IPOPT object that directly links to MATLAB. This object accepts exact first and second derivatives and exploits the full capabilities of IPOPT. Testing of this interface is currently underway.
- **ROMeo** – Recently, **David Ternet** of Simulation Sciences developed an interface between IPOPT and ROMeo, a widely used process modeling and optimization tool for real-time applications. IPOPT is currently being tested and compared with the current OPERA package by **Maame Poku** on a number of large-scale process problems. While ROMeo provides only provides exact first derivatives, it works well with the limited memory BFGS option in IPOPT.

In addition, **Yi-dong Lang** has developed a user-friendly version of dynamic optimization methods. In particular, they have extended these codes to exploit sparsity and are using them to tackle dynamic optimization problems including batch polymerization, crystallization and parameter estimation. This software, called *DynoPC,* runs under

Windows with a GUI interface. It has been distributed to several CAPD members and can now be downloaded on the same website as IPOPT. Currently, this approach is being extended to include parameter estimation problems, including the evaluation of confidence regions. This package, as well as IPOPT will be enhanced further by the development of a number of interfaces to optimization modeling platforms including CAPE-OPEN. A paper that describes this work is listed below.

Ignacio Grossmann's Group has been involved in the following developments:

In the area of optimization **Nick Sawaya** has been working in the development of cutting planes for nonlinear disjunctive problems and examined the issue of handling of the nonlinear constraints for the convex hull reformulation. **Lorena Bergamini** has completed the manuscript on the new method for the global optimization for the logic-based OA method that relies in the use of piecewise linear underestimators. **Aldo Vecchietti**, has continued to expand the capabilities in LOGMIP, a GAMS-based code for disjunctive programming (http://www.ceride.gov.ar/logmip/). **Ashish Agrawal** has addressed applied concepts of Type Theory for the formal specification of State-Task Networks.

In the area of process synthesis **Ramkumar Karuppiah** has started a new project on the synthesis of integrated process water systems for which he has developed a new global optimization algorithm that combines spatial search with piecewise linearization. In a joint collaboration project with BP, **Carlos Mendez** completed the superstructure optimization of a crystallization process for the separation of paraxylene. In a joint collaboration project with **Mike Domach, Soumitra Ghosh** has been developing screening strategies for NMR analytes for determination of metabolic flux maps using global optimization techniques. **Jose Caballero** in Alicante has developed a computational approach based on disjunctive programming and using process simulators for the design of distillation columns.

Vikas Goel is completing the implementation in C++ of a Lagrangean based branch and bound method for solving multistage stochastic programs in which the scenario trees are dependent of the design decision. He is applying this technique to the planning of gas fields. **Christos Maravelias** has shown that the discrete time STN model can be derived as a particular case from the continuous time MILP model that he developed in his Ph.D. thesis, and has produced a manuscript on this topic. **Muge Erdirik** has initiated a new project in the area of simultaneous planning and scheduling for continuous multiproduct plants in which she has developed a decomposition scheme that makes use of aggregation combined with logic cuts.. **Carlos Mendez** has been writing a comprehensive review paper in the area of batch scheduling. **Pedro Castro** has been investigating various formulations for the single stage problem with parallel units, and has found a novel RTN MILP formulation that performs as efficiently as the hybrid MLP-CP model by Jain. **Gabriela Garcia** has added the resource-constrained version of the new development problem (PRODEV) in the library of web-interfaces (http://newton.cheme.cmu.edu/interfaces)

Steinar Hauan's Group

John Siirola (co-advised by Art Westerberg) is nearing the end of his Ph.D. work on creating an agent system for distributed design and optimization. His latest work has been labeled "Polymorphic Optimization" and demonstrates how the simultaneous use of multiple models representing the same physical systems improve both solution quality and speed. The method has been applied to a microfluidic circuit design problem and was presented at the recent AIChE meeting.

Adesola Amosun, also working with agent system design, has demonstrated how performance may be improved by predictive control of resources during the agent system operation. The basic idea comes from a (time-dependent) Markov process and the system uses training data from previous runs to generate a probability transition matrix for favorable moves.

Anton Pfeiffer has completed his work on model formulation and solution approach for design of multiplexed microfluidic circuits where performance, layout and routing of i/o ports are considered simultaneously. The results were presented at a recent conference on circuit design (ICCAD '04); Anton will spend the spring semester doing an internship at CFDRC Corporation.

Xiang He -- working on design of microscale reaction-mixing systems -- has been comparing her plug-flow reactor network simulation model with both finite element approaches as well as more general methods for converting PDEs to ODEs. The PFR network model gives reasonable results and good solution times for most conditions, but encounter discrectization problems for systems with sharp fronts. Extensions to dynamic systems ("slug-flow reactors") are being developed based on finite difference approximations.

Mike Bartkovsky (experimental focus) and Jane Valentine (modeling focus) continue their work on MEMS-based biosensors. Mike has spent most of the fall semester designing and verifying the physical layout of the next generation membrane chips as well as integrating the first set of signal processing components. Jane has developed a perturbation method for analyzing system sensitivity with respect to asymmetrically placed, distributed binding regions.

Murni Amhad is designing flowsheets for protein separation by liquid-liquid extraction in the presence of contaminants. Preliminary work on incorporating the effects of ionic strength (through salts) has been completed and is being tested for robustness.

Israel Owusu has developed and implemented a framework for distributed, asynchronous simulation of Enterprise Resource Networks and has started testing on optimization of a simple set of supply chain units.

Gary Power's Group

The Powers' research group continues to work on the verification of chemical processing systems. Ph.D. candidate Calvin Chan is developing a library of unit models that will enable the rapid modeling of complex processing systems. The models include processing equipment, human operating procedures and control systems including software.

Calvin has recently presented results on the use of these methods for the verification of a chlorine vaporization system. This vaporization system clearly illustrates the need to consider the interactions between the equipment, control system and human procedures when assessing the safety and reliability of a process.

Denny Jacob recently joined our group as a Masters candidate and will be modeling and verifying the procedures for hydrotesting equipment used in off shore oil platforms.

Dr. Dan Milam is continuing his post doctoral work in Prof. Ed Clarke's group in the Computer Science department here at CMU. He is showing that the analysis of complex real time code written in C is now possible. This progress is important as the verification of the control code in many of our processes was a weak link in the safety and reliability analysis.

The models developed in this type of analysis are useful for the safety and reliability analysis of processes during design and serve as an important bench mark for change control during process modifications during start up and during process revisions and upgrades.

STATUS OF RESEARCH PROJECTS

Larry Biegler's Group

General Frameworks for Large Scale Optimization Strategies and Applications

Researcher: Carl Laird (Ph.D. started Fall, 2001)

As a result of several generations of Ph.D. students, we now have a general strategy for very efficient NLP algorithms including rSQP, full-space SQP, parameter estimation, data reconciliation and multiperiod optimization. Our most recent advance is in IPOPT, developed by Andreas Waechter. This code has become a core algorithm for

many of the research projects described below. In particular, Carl Laird has applied IPOPT and the AMPL interface to develop a novel source detection strategy for municipal water networks as an important application for barrier methods. This optimization problem is developed to detect attacks on networks and to determine optimal control and remediation strategies. Such networks are typically over several hundred to many thousands of nodes and require the incorporation of both spatial and temporal behavior. This difficult problem was reformulated as a DAE system with time delays. Moreover, because the hydraulic equations could be decoupled from the species mass balance, a novel preprocessing strategy renders the nodal constraints to be *linear* and the resulting problem can be solved easily using our simultaneous optimization strategies for dynamic optimization (see below). By exploiting the structure of these networks, discretized problems that represent actual municipal networks with up to 300,000 variables could be solved in only a few CPU seconds. An extension of this work that considers moving window strategies has recently been developed as well. A paper that describes this apporach is listed below. Finally, Carl spent the summer with Andreas Waechter at IBM to develop the next version of IPOPT. Designed in C++, this code is object oriented and flexible to deal with a wide variety of linear solvers, new barrier algorithms, and a variety of globalization strategies and decomposition approaches. Moreover, as noted above, the new code, IPOPT 3.1, provides a much easier interface to modeling environments.

Barrier (Interior Point) Methods for Nonlinear Programming

Researchers: **Maame Poku (Ph.D. started Fall, 2000)**
Carl Laird (Ph.D. started Fall, 2001)

This project considers an efficient strategy for solving nonlinear programs using interior point (IP) methods, developed by Andreas Waechter, currently at IBM Watson. The resulting approach works either in the full space or can take advantage of the particular reduced space decomposition strategies that we have developed in previous work. The advantage of this approach is that it solves the nonlinear problem directly without first exploring the solution of the QP subproblem. In this way we avoid the overhead in solving highly constrained QPs, as these have the same level of combinatorial complexity as the original NLP problem.

Andreas developed and tested a number of variations to this approach that include the use of line search approaches, decoupling the barrier terms from the reduced Hessian approximation and options for both primal and primal-dual barrier terms. Along these lines, Andreas has discovered that Newton-based IP methods that are applied directly to NLPs can experience convergence failures. These failures are analogous to infeasible QPs that can be encountered in SQP but are much more subtle because the cause cannot be detected easily. In particular, Andreas has developed a counter-example that illustrates this problem, and has also developed a through analysis of this difficulty. In addition, Andreas has developed an improved line search algorithm that is based on a recently developed *filter* approach. This approach overcomes this convergence difficulty and Andreas has completed a rigorous convergence analysis of his approach. Numerical testing on thousands of test problems has also shown some significant performance improvements over other barrier algorithms. Major features of this approach are:

- an implementation that allows either full space or reduced space options for the barrier NLP. In particular, the reduced space option has been tailored to the structure of DAEs solved with collocation on finite elements.
- a filter line search approach that replaces the classical merit function for line searches
- a preconditioned conjugate solver for the null space step that replaces quasi-Newton updating and uses true second order information instead of just quasi-Newton information.
- an open source license has been prepared for this code. The current version of this code can be downloaded from: http://www.coin-or.org.

The IPOPT code is being widely used in Larry's group and elsewhere. Examples include both full space and reduced space versions for dynamic optimization, in OCC and DynoPC, respectively. In addition, the full space approach is used in blending applications and in the solution of MPEC problems. Here**, Maame Poku** has applied IPOPT with the AMPL interface to deal with nonlinear planning and blending problems. These problems have a large number of

superbasic variables (degrees of freedom). As a result, reduced space NLP algorithms (like rSQP, MINOS, CONOPT and SNOPT) do not work well. Extensive results show that the full-space version of IPOPT works quite well on these problems. A paper that summarizes this approach is listed below. **Maame Poku** is currently applying this approach to data reconciliation and real-time optimization problems in SimSci's RomEO environment and is testing it on a number of large-scale real-time optimization problems.

Mathematical Programs with Equilibrium Constraints (MPECS)

Researchers: **Arvind Raghunathan (Ph.D. completed March, 2004)**
Prof. Ricardo Perez (Pontifical University of Chile)
Brian Baumrucker (Ph.D. started Fall, 2004)

MPECs represent an exciting new field in mathematical programming. While applications of MPECs have long been recognized in game theory, transportation planning, economics and engineering design, little work has been done in developing efficient algorithms for their solution In process engineering, these problems stem from bilevel and multilevel optimization problems as well as optimization of hybrid (discrete and continuous) systems. Included in this class are optimization problems with phase equilibrium constraints, as in equilibrium stage processes.

The MPEC problem is essentially a nonlinear programming problem augmented by complementarity conditions. The addition of these conditions leads to a violation of convergence assumptions for most nonlinear programming algorithms (e.g., linear independence of the constraint gradients) and can cause these algorithms to fail. On the other hand, the barrier method described above has a straightforward extension to these problems. As a result, complementarity constraints can be incorporated with little additional cost in the algorithm. In fact, all of the features that contribute to the efficient performance of IPOPT can be invoked directly for the solution of the MPEC problems. The resulting algorithm based on IPOPT has been developed further and refined for a number of challenging dynamic optimization applications in process engineering. Our work in this area includes the following:

Arvind Raghunathan recently completed his Ph.D. and has accepted a position with United Technologies. In his research, he has incorporated the MPEC formulation into the IPOPT code, now called IPOPT-C, along with algorithmic modifications to treat the complementarity constraints more efficiently. This code has been interfaced to the AMPL modeling system and has been tested on a set of library MPEC problems. Our results show that this implementation compares well against competing barrier algorithms such as LOQO.

Arvind tested this approach on a number of process optimization problems with phase equilibrium constraints. These include distillation optimization problems with disappearing vapor and liquid phases on equilibrium stages, dynamic systems with switching conditions, such as overflows and phase disappearance in distillation columns and metabolic network systems. For the latter, we have considered parameter estimation problems for dynamic fermentation systems for wine production. These results show that this approach leads to better and more uniform performance than the smoothing approach used in our previous studies.

Future work deals with modeling and optimization of dynamic biological systems that are based on cellular models. Such systems are large-scale extensions of MPECs. Moreover, they have interesting modeling features since state dependent constraint functions with discontinuities also need to be treated through MPEC formulations. Finally, a recent project with IBM, involving Andreas Waechter and Andy Conn, is exploring the suitability of MPEC formulations to solve mixed integer nonlinear programming problems. Brian Baumrucker has recently joined the group and will be considering the developing of good MPEC formulations that model discrete decisions.

Simultaneous Optimization of Differential-Algebraic (DAE) Systems

Students: **Juan Arrieta Camacho (Ph.D. started Fall, 2002)**
Shivakumar Kameswaran (Ph. D. started Fall, 2001)
Victor Zavala (Ph.D. started Fall, 2004)

Visitors: **Antonio Flores-Tlacuahuac (University of Iberoamericana, 2004)**
Yi-dong Lang (Jiansu Research Institute, Nanjing, China)

This topic on simultaneous solution and optimization strategies for large-scale, dynamic optimization problems incorporates a number of projects. In the past, we have applied this approach to optimization problems for batch reactors, process dynamics and tray-by-tray batch distillation and large-scale dynamic flowsheeting models. Moreover, we have tackled dynamic examples successfully with this approach that cause any sequential dynamic optimization method to fail. This is due to the possible presence of unstable modes in the forward direction as well as the exact treatment of path constraints. It can occur in open-loop unstable systems that arise in optimal control and nonlinear MPC, dynamic parameter estimation and the optimization of runaway reactors. Prof. Antonio Flores, a sabbatical visitor from the University of Iberoamericana, has demonstrated the advantages of this approach on a number of challenging polymerization processes. Moreover, he has recently extended this to consider the design of control systems for potentially unstable processes. A paper that describes this approach is listed below. Finally, this approach can also be integrated into a two level optimization strategy that alternately solves the dynamic optimization problem for a fixed mesh, and then optimizes the mesh in an outer level; it easily allows for the addition of moving finite elements as well. A number of research projects have are currently being addressed in our group.

Dynamic Optimization Platforms

We have developed two complementary modeling frameworks for dynamic optimization, one based on reduced space and one on full space. First, over the past four years Yi-dong Lang has developed a stand-alone Windows modeling system for dynamic optimization called ***DynoPC***. Written for Windows with a Visual Basic user interface and with heavy integration of graphical, simulation and automatic differentiation tools, this software package incorporates our advances in dynamic optimization, particularly IPOPT and the elemental decomposition. This program continues to be distributed to interested research groups both in academia and industry and can be downloaded from http://coin-or.org Current developments with DynoPC include a collaboration with Prof. Marquardt's group at the Technical University at Aachen (RWTH). Here we have incorporated ESO interfaces that are compliant with recently developed CAPE-Open protocols. This leads to an interface compatible with a number of existing process models and modeling environments. In particular, Yi-dong has recently completed a polymer reactor study that was modeled in gProms and solved with DynoPC. This problem had over 300,000 variables and was solved in about an hour of CPU time. Further reformulations of this system, using a simple partitioning strategy, have led to an optimization problem that is much better conditioned and can now be solved in only about 1000 CPU secs. A paper that describes this approach is listed below.

Second, we have been using IPOPT in a full space framework linked to the AMPL modeling environment. As detailed in many of the studies listed below, this framework has been extremely powerful and flexible in solving a wide variety of problems. However, there are a number of limits to problem sizes that can be considered with this strategy. As a result, updates to IPOPT also need to be transferred to reduced space optimization strategies. We are currently adopting a MATLAB framework and coupled it with the AMPL modeling language. Domain specific prototypes have already been developed (as described below) and work very well.

Consistency and Convergence of Simultaneous NLP Formulations for Dynamic Optimization

Does the solution of the discretized NLP converge to the solution of the original optimal control problem? What are the particular problem classes and assumptions for which this can be shown? This has been an interesting and long-standing research problem. Back in 1989, we have developed some consistency results based on the work of Reddien for Gauss collocation schemes. In addition, Lagrange multipliers from the KKT conditions have a direct relationship to adjoint variables from the Euler-Lagrange equations. However, more powerful convergence results are difficult to show and usually apply only to well-conditioned linear-quadratic control problems. Nevertheless, despite limited convergence results, very good performance is usually obtained with simultaneous optimization strategies.

Recently, Shiva has revisited some of the theory in order to derive properties for Radau and Lobatto collocation. Both of these methods (while of lower order) tend to behave much better than Gauss collocation. We have recently derived order conditions for these methods and have related their convergence properties to the more general class of boundary value solvers. Moreover, these have been verified by a number of example problems. A manuscript that discusses these results will appear with the next newsletter. Moreover, these results points to the solution of singular control problems. These features lead to ill-conditioned KKT matrices, nonunique solutions and possible failure of

the NLP solver. Based on the convergence analysis, we intend to develop reformulations that will regularize the KKT matrix and provide a consistent theory for more general optimal control problems. Finally, in tandem with work by John Betts at Boeing and Prof. Steve Campbell at NC State, we have considered an analysis of high index path constrained problems. This analysis shows that the simultaneous approach leads to much better conditioned problems that those based on classical optimal control. A paper that discusses these properties in detail is listed below.

Nonlinear Model Predictive Control Strategies

Through collaborations with D. Subramanian and T. Samad at Honeywell, Inc. Arvind Raghunathan had been pursuing an important research problem on conflict resolution of aircraft trajectories. Given a set of aircraft with starting points, destinations, protection zones and obstacles, what are the optimal trajectories that lead to the best performance or minimum fuel consumption? Moreover, detailed flight models are employed that limit the maneuverability of these aircraft. This problem leads to a nonconvex dynamic optimization problem. Moreover, protection zones lead to disjunctive constraints that have been modeled through convex hull formulations. The resulting problems are discretized using collocation on finite elements and solved using IPOPT. A reprint that describes this approach and demonstrates excellent performance on this problem is listed below. In particular, this approach was incorporated into a flight demonstration package called CROMA (Conflict Resolution of Multiple Aircraft), which combines IPOPT and AMPL within a MATLAB interface. As a result large problems with up to 8 aircraft and 4 obstacles have been solved efficiently.

Our current work extends these off-line CROMA strategies to on-line nonlinear model predictive control (NMPC). Here only partial solutions are considered for the aircraft trajectory and efficient NLP solutions are required in order to guarantee on-line performance and stability. Juan Arrieta has recently developed two prototype formulations: an NMPC strategy based on a detailed NLP solution and an MPC strategy based on solutions of QPs. Both of these strategies have demonstrated efficient partial solution strategies that allow conflict free flight in the face of many aircraft and obstacles. In particular he has shown that the NMPC strategy does no suffer from large deviations from the optimal trajectory in the nominal case; it has handled pop-up threats and incorporates limitations due to radar ranges. Juan has also extended this approach to a number of more complicated aerospace models including satellite trajectories and NMPC variations of these trajectories. His recent work has shown that our approach generates optimal solutions significantly faster than competing methods. A paper that describes this approach is listed below.

The NMPC strategy is also being extended to large-scale models for polymerization processes. In a project funded by ExxonMobil Chemicals, Victor Zavala has begun to develop multi-stage dynamic optimization problems for grade transition and defouling operations.

Large-Scale Optimization for Fuel Cell Models

Researchers: Cong Xu (Ph.D. student started Fall, 2000, joint with Prof. M. S. Jhon)

Cong Xu has been investigating optimization problems arising in fuel cell applications, including Direct Methanol Fuel Cells (DMFCs) and Hydrogen PEM fuel cells. In particular, he has extended simple DAE models for fuel cells to consider optimal flow patterns and minimization of contamination effects due to membrane crossover, and he has extended these models to consider sensitivity and optimization calculations. In particular for DMFCs, Cong Xu and Peter Follmann have compared and critically assessed several literature models and have explored the crossover phenomenon. By applying our dynamic simulation and optimization tools, they were able to develop dynamic feeding strategies for these systems that greatly reduce contamination due to methanol crossover. These systems have been modeled and optimized with a variety of FORTRAN, MATLAB and MAPLE-based tools, such as OCC. The results show that the optimal design of DMFCs can be achieved without pulsed operation. Here crossover is significantly reduced and the power density is correspondingly increased. Cong's current work deals with the optimization of hydrogen fuel cells and the incorporation of ancillary process models. The efficiency of these processes can also be improved through flowsheet optimization strategies as well as heat integration of the process units. This approach is based on conventional flowsheet optimization schemes within Aspen/Plus along with simultaneous optimization and heat integration strategies. The application to fuel cell based processes leads to interesting trade-offs between the fuel cell, the rest of the flowsheet and the heat recovery system.

Optimization and Control of Pressure Swing Adsorption Systems

Student: **Yoshi Kawajiri (Ph.D. started Fall, 2003)**
Seth Knaebel (MS completed Summer, 2004)

Visiting Researchers: **Vanesa de la Torre (PLAPIQUI)**
Daeho Ko (Yonsei University)
V. Grant Fox (formerly Air Products)

In tandem with dynamic optimization projects, we are also developing more direct sequential strategies for the solution of dynamic optimization problems. These sequential approaches are easy to construct and have seen a lot of previous development in other research groups. An important (and time-consuming) aspect to these sequential strategies is obtaining sensitivities from the dynamic model efficiently. Fortunately, recent projects by Barton at MIT, Petzold at UC-Santa Barbara, and researchers at the Max Planck Institute have led to excellent software implementations that calculate sensitivities efficiently from large DAE process models. Also, these sequential approaches take advantage of 'off-the-shelf' solvers and do not require a heavy research investment as with simultaneous methods. As a result, we are embarking on large-scale dynamic optimization projects that combine our large-scale rSQP tools with efficient DAE solvers and sensitivity codes. One interesting benefit of this approach is that the most time-consuming elements can easily be parallelized with linear speedups.

To take advantage of these algorithms, we have completed a NSF/GOALI initiative with Air Products for the optimization of Pressure Swing Adsorption (PSA) systems. For this approach we have exploited existing models and implementations for the optimization of comprehensive, detailed PSA systems. Up to now, no satisfactory optimization strategies have been developed that can deal with these models. In her Ph.D. thesis, Ling Jiang has generated a number of interesting results for this project. She has been spending her summers at Air Products to apply sophisticated sensitivity codes, like DASPK 3.0, and automatic differentiation codes, like ADIFOR, to adsorption bed models created from the method of lines. In particular, she concentrated on developing detailed PSA bed models with hyperbolic and parabolic components that require special mass conserving discretization strategies to convert them to DAEs. Termed flux limiters, these discretizations allow the accurate tracking of steep fronts and discontinuities that frequently arise in PSA systems. Ling has successfully simulated and optimized cyclic steady state conditions for two PSA units, using Newton-type and tailored rSQP solvers. From this point she has demonstrated a framework that includes constrained simulation problems and design optimization problems on a number of PSA examples. *Preliminary results of her work show that this optimization strategy can reduced the power requirements for PSA systems by about 15% and the computational cost is an order of magnitude less that with conventional case study approaches* .More recently, she has implemented this approach to run in parallel on our Beowulf cluster; this leads to tremendous speedups in PSA optimization, as the sensitivity equations are trivial to parallelize. Finally, this work has been applied to complex PSA systems for the separation of high purity hydrogen from refinry gases. A reprint that describes this work is listed below.

In addition, we are extending this PSA optimization strategy to a number of more complex systems, as follows.

- First, these systems are used for the sequestration of CO2 from flue gases. Previous work by Dr. Daeho Ko has shown that efficient optimization formulations can be developed in gProms. Dr. Ko is continuing this work with researchers at NETL in order to develop new sorbents for PSA and TSA operations for CO2 recovery. A paper that describes this approach is listed below.
- The gProms models are also currently being extended to separations of H2 and CH4 by Seth Knaebel, who recently completed an MS thesis. He has modified these models with new isotherm data and also evaluated and optimized of a number of new PSA cycles. This work is described in a paper listed below.
- Vanesa de la Torre is developing optimization models for PSA systems that address load following approaches induced by changes in product demand. These models will be used to develop MPC strategies for on-line control of a number of PSA processes.

Data Reconciliation for Steady State and Dynamic Processes

Researchers: Nikhil Arora (Ph.D. started January, 1999)
Shivakumar Kameswaran (Ph.D. started Fall, 2001)

Previously, Nikhil Arora (now with PraxAir in Tonawanda, NY) extended data reconciliation and parameter estimation strategies to both steady state and dynamic processes. Initially, he applied statistical tools to determine steady state conditions, classify measurements and observed model variables, detect data outliers and estimate model parameters. Nikhil has also developed specialized algorithms that deal more efficiently and reliably with these problem classes. In particular, he applied bounded trust region strategies to deal with problems that are overparametrized and likely to have nonunique solutions. Our results with this algorithm, called NTREST (Nonlinear Trust Region Estimation), have shown that these approaches are more reliable than and just as efficient as general-purpose NLP strategies. These are currently being incorporated within a large scale SQP framework as well to take advantage of rapid convergence. This approach is currently being extended to EVM problems as well. Moreover, this algorithm was applied to a challenging parameter estimation problem arising from a polymer reactor model. Applied to a number of cases, Nikhil was able to determine solutions to a variety of poorly conditioned parameter estimation problems. Two reprints that describe this approach are given below.

In a project sponsored by Exxon Upstream Research, Shivakumar Kameswaran has taken over this project and is working on system identification and parameter estimation for oilfield applications. Using IPOPT and AMPL as a dynamic optimization tool he is studying parameter estimation for distributed parameter systems that are potentially ill-conditioned. Here the permeability field needs to be determined using data taken from core samples extracted from reservoirs. Knowledge of this field allows the development of flooding strategies for optimal oil extraction. Moreover, the reservoir model contains a number of interesting features including complementarity relations for capillary pressure and multivariate measurements. Shiva has formulated this problem as a large-scale MPEC and obtained very efficient results. These results have also been validated with actual core data. This is currently being extended to large-scale history matching problems for reservoir models. Also, these models are currently being converted into an AIMMS format and will be solved through the new interface to IPOPT.

Ignacio Grossmann's Group

Algorithms for Nonlinear Disjunctive Programming

Student: **Nicolas Sawaya [Ph.D., started Jan02]**
Visitor: **Lorena Bergamini [Ph.D. Jan 03]**
Research collaborator: **Aldo Vecchietti [Researcher at INGAR]**
New Developments: **Cutting plane method for branch and bound MINLP**

Nicolas Sawaya

The objective of Nick's project is to develop novel solution methods for nonlinear generalized disjunctive programs (GDP). There are two major issues that arise in the continuous relaxation based on the convex hull for linear or nonlinear problems: (a) the corresponding formulations may lead to a problem of large size due to the disaggregation of variables; (b) the corresponding relaxation may produce a lower bound similar or equal to the one obtained from the big-M reformulation of the GDP. One objective in Nick's work has been to develop effective cutting plane methods for linear GDP problems. The other objective has been to develop an integrated framework for solving nonlinear GDP problems.

The first major step in Nick's research work was to develop a solution method for linear GDP problems that relies on cutting planes, and that can generally be embedded within a branch and cut algorithm. The major steps of the algorithm are to first solve the big-M relaxation. Next, we formulate and solve a separation problem in which we minimize the difference between a feasible point in the convex hull relaxation and the solution of the big-M problem. Here we can use the 1, 2 or infinity norm, with the first and last leading to linear objectives. If the difference in the separation problem is small or even zero this is a clear indication that the both the big-M and the

convex hull relaxations are essentially identical. If, on the other hand, the difference is not small this not only tells that the convex hull formulation is tighter, but one can derive a cutting plane, which for the linear case corresponds to a facet of the convex hull. The derivation of successive cutting planes continues until the improvement in the lower bound of the big-M model with the cutting planes lies within a tolerance. The idea is then to switch to a branch and bound method. Nick has developed a nice theoretical derivation of the cutting planes for the 1, 2 and infinity norms based on the use of subgradient optimization.

Nick applied his cutting plane technique to three major problems using the infinity norm. The first is the strip packing problem that consists of fitting a set of rectangles in a roll of fixed width in order to minimize its length. The largest problem that Nick solved involved 21 rectangles. The convex hull formulation is significantly larger than the big-M model (5272 vs 1072 constraints, 4244 vs 884 continuous variables; both have 840 0-1 variables). The big-M formulation required 1 416 137 nodes and a CPU-time of 4093 with CPLEX 8.1. The convex hull formulation required 968 652 nodes in a time limit of 10 800 secs in which the problem was not solved to even feasibility. In contrast with 60 cutting planes the number of nodes was reduced down to 28611 nodes and 79 seconds! It should be noted that these times include the times for solving the separation problem. Nick also solved 10 process retrofit problem, and extension of a model that Jennifer Jackson formulated, and he also addressed a job-shop scheduling problem with up to 10 jobs and 8 stages. The cutting plane technique was not very helpful in both cases, although in the retrofit problem it did improve substantially the performance of the big-M reformulation.

Nick has also investigated the use of cutting planes for solving nonlinear disjunctive problems. A major issue here has been to revisit the nagging problem of how to implement the constraint $\lambda\, g(\nu/\lambda)\leq 0$ for the case when λ goes to zero. In our previous work we had used the simple approximation $(\lambda+\varepsilon)\, g(\nu/(\lambda+\varepsilon)\leq 0$ This however can give rise to problems depending on how ε is selected. Nick has proposed a new approximation given by $(\lambda+\varepsilon)\, g(\nu/(\lambda+\varepsilon)\leq \varepsilon g(U)$ which has the nice property that it holds for both when λ goes to zero and non-zero. Nick has successfully tested this approximation on a number of test problems setting ε to 0.00001. Nick has also studied the generation of cutting planes for nonlinear GDP problems that are reformulated as big-M MINLP's and solved through branch and bound. Nick has tested this method on a batch design problem with intermediate storage. The convex hull reformulation involved 1296 constraints, 637 continuous variables and 89 0-1 variables. In contrast the big_m model only involves 800 constraints, 239 continuous variables and 89 0-1 variables. The convex hull formulation was solved in 711 secs enumerating 5 359 nodes. The big-M formulation was solved in 787 secs enumerating 12 449 nodes. The NLP relaxations were 650,401 and 641,763, respectively. With the proposed cutting plane method, using the infinity norm, the NLP relaxation of the big-M was increased to the one of the convex hull with 58 cutting planes. In that way the number of nodes was reduced to 7 528, and the required time to 610 secs (including 8.7 secs for the cut generation). Thus, the proposed cutting plane led to good improvements. Nick plans to unify the application of cutting planes to the different solution methods for GDP. Finally, Nick is also starting to build a library of convex MINLP problems that will be used in a new collaboration with IBM that involves Larry Biegler and Gerard Cornjuelos from the Tepper Business School.

Lorena Bergamini

Lorena, a Ph.D. student from INGAR in Argentina working under the direction of Pio Aguirre and who spent one semester with us, developed a new deterministic algorithm for the global optimization of process networks that are formulated as Generalized Disjunctive Programs and that involve nonconvexities. The global optimization algorithm relies on the use of piecewise MILP approximations (no spatial branch and bound search). Also, the method is based on the Logic-Based Outer Approximation (OA) algorithm developed previously by Metin Turkay and that overcomes difficulties related to singularities that are due to zero flows. The method developed by Lorena is capable of handling nonconvexities, while rigorously guaranteeing the global optimality of the synthesis of process networks. This is accomplished by constructing a master problem that is a valid bounding representation of the original problem, and by solving the NLP subproblems to global optimality.

Lorena assumed that the functions involved are sum of convex, bilinear, and concave terms. The logic-based OA algorithm consists of an iterative procedure in which the problem is decomposed into continuous and discrete optimization subproblems. The continuous optimization subproblem requires the solution of reduced NLP subproblems, which are obtained by fixing the Boolean variables, while the discrete optimization is obtained through the solution of MILP master problems. In order to rigorously maintain the bounding properties of the MILP

master problem for nonconvex problems, piecewise linear under and overestimators for bilinear, and concave terms are constructed over a grid with the property of having zero gap in the finite set of points. The set of these approximation points are defined over subdomains defined by bounds of variables and solution points of the previous NLP subproblems. For bilinear terms, the convex envelope by McCormick is used. Disjunctions are used to formulate the convex envelope in each subdomain, and the convex hull of these disjunctions is used to provide the tightest relaxation. Note that binary variables are needed for the discrete choice of the corresponding subdomains. Linear fractional functions are treated in a similar way. Piecewise linear subestimations replace the concave terms. The NLP subproblems are also solved to global optimality using a reducd MILP master problem. Since the NLP subproblems are reduced problems, involving only continuous variables related to a process with fixed structure, the variable bounds can be tightened thereby enhancing the understimators. Lorena has applied this algorithm on a number of different problems. For instance, the algorithm has been applied in a process network problem that originated in an internship of Sangbum Lee at Eastman Chemical and that involves 17 Boolean variables, 973 continuous variables and 725 constraints. The algorithm required 5 minutes, while BARON could not solve the problem within 15 minutes. Lorena has alos applied the method to a heat exchanger network with two hot and two cold streams (16 boolean variables, 82 continuous variables, 16 disjunctions, 112 constraints) requiring 59 secs to find the global optimum. In contrast, BARON required almost 20 minutes. Lorena has completed a manuscript on this work which has been submitted for publication.

Aldo Vecchietti: LOGMIP and modeling issues

Aldo and his students at INGAR in Argentina are developing the LogMIP code, which is as an extension of the GAMS modeling language for posing logic/disjunctive problems. The main features of LogMIP are several language constructs in order to concisely formulate GDP problems. The syntax developed involves the use of IF THEN ELSE statements to represent the disjunctions, including embedded ones. An interesting related development has also been to show that logic constructs that are commonly used in Constrained Logic Programming (CLP), such as implications for constraints (e.g. $g(x) \leq 0 \Rightarrow f(x) \leq 0$) can be systematically converted in the form of disjunctions. The intent is also to be able to accommodate hybrid models that are partly expressed as disjunctions and partly as equations in algebraic form.

Aldo has completed in LogMIP the definition of disjunctions over sets and subsets. The conditional statement operator WITH in conjunction with other operators: relational operators (<, <=, =, >, <=), logical operators (and, or) and sets operators (ord, card, in) or using a subset definition are used to control de disjunction's domain defined over a set. An example, which previously required specifying the disjunction for each subset element, is given below where it can be seen that only one statement is required for defining the disjunction:

```
SET  I  jobs   / A, B, C, D, E, F, G / ;
ALIAS(I,K);
SET  J  stages / 1*5 /;
ALIAS(J,M);
SET L(I,K,J) / A.B.3,  A.B.5,  A.C.1, A.D.3, A.E.3, A.E.5, A.F.1, A.F.3, A.G.5, B.C.2, B.D.2, B.D.3, B.E.2, B.E.3,
B.E.5, B.F.3, B.G.2, B.G.5,   C.D.2,  C.D.4,  C.E.2,  C.F.1,  C.F.4, C.G.2, C.G.4,
D.E.2, D.E.3, D.F.3, D.F.4, D.G.2, D.G.4, E.F.3, E.G.2, E.G.5, F.G.4 /;
DISJUNCTION D1(I,K,J);
D1(I,K,J)
      with (L(I,K,J)) IS
IF Y(I,K,J) THEN
      NOCLASH1(I,K,J);
ELSE
      NOCLASH2(I,K,J);
ENDIF;
```

As for the propositional logic, the special constructs ATLEAST, ATMOST, EXACTLY are defined to specify that the sum over a subset of variables with a given cardinality is at least, at most or equal to one. Also, LogMIP can now accept logic propositions in symbolic form without the need of translating them into linear inequalities. Logic propositions are used to establish relationships between disjunctions terms. The operators defined for writing these sentences are:

Symbol	Meaning
->	Implication
<->	equivalence
not	negation
and	logical and
or	logical or

For example:
Y('1') -> Y('3') or Y('4') or Y('5');
Y('3') -> Y('8');
Y('3') -> Y('6') and Y('9');

For solving linear disjunctive/hybrid problems LOGMIP can automatically generate the convex hull relaxation and big-M transformation for linear problems. Aldo has implemented LogMIP in the IDE version of GAMS and tested it with small and medium sized problems that include jobshop scheduling and the retrofit MILP model from Jennifer Jackson. For solving nonlinear disjunctive/hybrid problems Aldo has also automated the logic-based OA algorithm, which is suitable for nonlinear GDP process network problems. Future work will involve the implementation additional nonlinear algorithms. As for the more impressive numerical results with LogMIP, in one of Jennifer's models, Aldo found that the big-M formulation of her retrofit planning problem takes about 1745 nodes with OSL, while convex formulation through LOGMIP only requires 9 branch and bound nodes!.
LogMIP Website is now also available, http://www.ceride.gov.ar/logmip/. The Website includes now some explanation about LogMIP, the User's manual, solvers and examples downloads, references and links.

Modeling and Optimization of Hybrid Systems for Supply Chain Problems

New developments: **Type Theory for State-Task Network**

Students: **Ashish Agarwal [Ph.D. , started Jan 02]**

The objective of Ashish's project is to develop a new hybrid systems framework for modeling supply chain networks. The basic idea in Ashish's project is to rely on a hybrid dynamic systems representation that combines differential equations to capture the continuous dynamics and automata to capture the discrete dynamics. Each automaton describes the space and dynamics of a single discrete variable. The continuous dynamics is used to represent material flow, while the discrete dynamics is used to model scheduling decisions. The hybrid dynamic representation is then applied to a supply-demand network in order to provide a formal representation of the system, determine the optimal operating conditions, scheduling deliveries, selecting between outsourcing and production, and performing a dynamic allocation of resources.

Ashish developed a representation based on automata than can be systematically transformed into one with finite states, then to a disjunctive programming model, and finally into a mixed-integer linear program. In this way an important accomplishment is that one can systematically derive the mixed-integer linear programming model describing the supply demand optimization network problem. Ashish has tested the model formulation on a small supply chain optimization problem demonstrating that the model can be expressed in very compact form. Ashish has completed a manuscript describing this work. He is also developing software written in ML that will allow to represent a hybrid system with his level representation and automatically convert it into an MILP problem.

Over the last few months Ashish has been investigating the use of Type Theory as a systematic formalism for proving correctness of formulations. The basic idea is to define the different variable and operator types so that all transformations of data or coefficients are "well-formed." In this way one can use such a representation as a basis for developing software that has a strong foundation, and that is more likely to be free of errors. Ashish has applied this formalism to the definition the classical State-Task Network, which can then be used to automatically generate the MILP model. Ashish is currently investigating the use of Type Theory to the definition of a hybrid system based on automata. As a first step this will involve the transformation from disjunctive to MILP form.

Optimal Synthesis of Integrated Process Water Systems

New developments: **Global optimization of NLP superstructure**

Students: **Ramkumar Karuppiah [Ph.D. , started Jan 04]**

Ram, a new student from IIT Dehli, successfully passed the Ph.D. qualifying exam. He has initiated this new project that deals with the synthesis of process water systems that integrate the water reuse section for processes with the distributed water treatment section for a given number of contaminants. The initial objective is to find for given sets of processes and given treatment units the optimal configuration of the system that minimizes the use of freshwater, or more generally minimizes the total cost. Ram has assumed for the processes units that they are either characterized by fixed contaminant loads, or by variable loads that obey mass exchange constraints in terms of concentrations. For the treatment units fixed recoveries are specified. The initial objective chosen has been to minimize the amount of freshwater and the amounts of water processed in the treatment units. More general cost objective can also be handled.

Ram has developed a superstructure that involves all possible alternatives for interconnection of process and treatment units, and mixing and splitting of streams. The corresponding model corresponds to an NLP model with bilinearities in the mixers given by the product of flows times concentrations in ppm of the contaminants. Ram has developed a global optimization algorithm that relies on combining spatial branch and bound search, with piecewise linear approximations inspired by the work of Lorena Bergamini. The motivation is that piecewise linearizations improve the quality of the lower bound, but they do it at the expenmse of introducing additional 0-1 variables. For this reason it would seem to be sensible to still use a spatial branch and bound search, but strengthened by piecewise linearizations for a fixed (modest) number of intervals. To also strengthen the quality of the lower bound, Ram has derived a valid cut that represents overall mass balances for each of the contaminants. The algorithm also relies on bound tightening and on branching only on the flows. The bisection rule was found to be the most effective for partitioning.

Ram has tested his method with several examples. In one containing 3 process units and 3 treatment units, the corresponding NLP involves 150 variables and 118 constraints (80 bilinear terms). CONOPT failed to solve the NLP from various starting points, and when it converged to a local solution, the best it found had an objective of 138.56 ton/hr (feedwater plus amounts water treated). The method of Ram converged to the global solution of 128.12 ton/hr requiring 7 nodes in the branch and bound tree and 54 secs of CPU-time. BARON was also used to solve this problem requiring 1807 nodes and 454 secs. In another problem involving 4 process units and 3 treatment units the NLP had 195 variables and 151 constraints. CONOPT either did not converge, or if it did, the best it found was 186.18 ton/hr. Our proposed method converged to the global optimum of 170.39 ton/hr, requiring only 10.3 secs solving the problem at the root node. BARON in contrast required 3490.5 seconds and 9656 nodes. Work is under way to extend the model to general cost functions and to variable number of treatment units which will lead to an MINLP model due to 0-1 variables that are needed to model these units.

Disjunctive Optimization Techniques for the Synthesis and Design of Separation Synthesis

New developments: **Tray-by-tray optimization design using process simulators**

Students: **Mariana Barttfeld (Ph.D. INGAR-graduated August 2003)**
Collaborators: **Jose Caballero [Associate Prof., Univ. Alicante]**

This project deals with a modeling framework for separation systems based on the State-Task Network (STN) and State Equipment Network (SEN) representations. These models are formulated with generalized disjunctive programming (GDP) models that explicitly handle discrete and continuous variables. The intent has been to develop rigorous optimization procedures that can make use of tray by tray models. Mariana Barttfeld from Argentina concentrated on MINLP and GDP models for single columns and complex column configurations. Jose Caballero in Spain is working on the analysis and synthesis of thermally integrated columns.

Mariana Barttfeld

Mariana stayed with Ignacio's group for one year in a collaboration with Prof. Pio Aguirre from INGAR in Argentina. She first performed a comprehensive comparison between MINLP and GDP models for optimal design of distillation columns in which several representation of the superstructure based on tray-by-tray models were used. Mariana coupled the MINLP and GDP models with an NLP thermodynamic initialization model that assumes that all the potential trays are present at the final solution. For the MINLP model, a reduction of candidate trays was performed to decrease the number of trays. From several ternary mixtures that she considered the most effective MINLP model proved to be case of variable feed and reboil location. For the GDP the case of fixed reflux, feed and reboiler trays, and all other as conditional trays, proved to be the best, which in fact is the representation that was used by Hector Yeomans. For the MINLP case convergence was only achieved with the initialization procedure. For the GDP case it helped, but it was less critical. In all cases the MINLP models took about one order of magnitude longer time than the GDP models. On the other hand the reduction scheme of the MINLP model produced lower cost solutions than with the GDP models due to a strategy for reducing candidate trays from the relaxation..

Mariana also investigated the synthesis of superstructures for complex column configurations (e.g. side rectifiers, side strippers) using tray-by-tray models that she studied for individual column design. The superstructure is based on the reversible distillation sequence model by Fonyo (1974) for which Mariana developed both STN and column superstructure representations, for both zeotropic and azeotropic mixtures. For the optimization of the superstructure she developed a decomposition method in which the basic idea is to consider first the selection of column sections, and next the selection of trays for the selected sections. A GDP model was first formulated, which is solved as follows. The NLP thermodynamic initialization is first solved with the maximum number of trays for all sections. This is then used to derive an MILP master problem (based on convex hull) for selecting the sections in the superstructure. This model then selects the sections for which another MILP is formulated for selecting the number of trays in the selected sections. The reduced NLP subproblem is then solved to obtain an upper bound to the cost. An integer cut is added and the corresponding MILPs are updated. These are then solved to generate new configurations based on sections, and number of trays. Mariana solved several problems including an example of an azeotropic mixture (methanol, ethanol, water). in which she used a superstructure with 5 columns. The GDP involved 210 discrete variables and about 10,000 continuous variables and constraints, and was solved in 64 minutes, yielding a two column configuration with side stripper and side extraction. The work by Mariana was recently presented at a plenary talk at the ESCAPE15 Conference.

Jose Caballero

In the past Jose has addressed the issue of systematically generating all the configurations for thermally coupled distillation columns, including those that are structurally equivalent. In addition, the goal is to identify structures that are "easy to control" in the sense that interconnections of the columns flow from high to low pressure. Jose developed a set of logic propositions that can be expressed as constraints in an GDP model to define the search space for these thermally integrated columns. Jose also derived equations to calculate the number of thermodynamically equivalent configurations for a given sequence of tasks.

Jose has developed a novel superstructure for synthesizing non-azeotropic mixtures with the Underwood-Fenske-Gilliland approximations. The synthesis approach considers alternatives from conventional sequences, in which each final distillation column has a condenser and a reboiler, to fully thermally coupled distillation sequences going through all possible intermediate combinations. In order to perform the optimization of the superstructure Jose formulated the problem as a disjunctive programming problem, and developed a two-stage solution procedure. In the first one a sequence of tasks is optimized, and then in a second stage the best configuration in actual columns is extracted among all the thermodynamically equivalent configurations. The model has proved to be robust and reliable. The more complex example involved 5 alcohols (ethanol, isopropanol, 1-propanol, isobutanol, 1-butanol). The optimal configuration involved 5 columns with 24 trays (AB/BCDE), 45 trays (BCD/E), 40 trays (BC/D), 120 trays (A/B) and (B/C) 29 trays. The CPU-time required was several minutes. Rigorous simulations in HYSYS showed very good agreement with results presented.

In his most recent work Jose has been investigating a strategy for determining optimal design of distillation columns using a process simulator (ASPEN) and using the disjunctive programming framework. A major motivation has been to avoid the need of explicitly handling the thermodynamic equations as has been the case in Mariana's work. The idea in Jose's model is to adopt the Logic-Based Outer-Approximation Method in which the NLP subproblem is given only by the existing trays in the column. For this Jose uses the optimization capability in ASPEN to optimize a column with fixed number of trays. In order to define the MILP master problem Jose performs numerical perturbations on the degrees of freedom (usually only two variables). In addition he performs a sequence of simulations by adding and deleting trays in each section in order to evaluate the economic potential of these decisions which are modeled as 0-1 variables in the MILP. This scheme has proved to be quite successful. So far largest problem that Jose applied it was to a mixture of 2-propanol, 1-propanol, i-butanol and 1-butanol. A column with 70 trays was postulated (feed in tray 35). The optimum was found in 3 major iterations. The design yielded a column with 27 trays (tray 24 to 57) and was solved in about 1 min CPU-time. Jose is finishing the testing of this method with few more examples. The manuscript should be available for the next newsletter.

Synthesis of Crystallization Processes

New developments: **Superstructure optimization for refrigeration system**

Post-doctoral fellow: **Carlos Mendez (started Janaury 2003)**

In a joint collaboration project with Jeff Logsdon, John Myers and Scott Roberts from BP, Carlos has been addressing the separation of paraxylene, orthoxylene and methaxylene through a crystallization process given that their boiling points are very close making the use of distillation unattractive. Carlos first developed an NLP optimization model for the operating and design optimization of a fixed configuration of a crystallization process for the separation for paraxylene. The process involves crystallizers, reslurry drums, centrifuges, heat exchangers and a refrigeration system. The model, which makes use of short-cut equations for predicting the mass and energy balances and sizes, is quite challenging to converge due to the nonlinearities involved. To circumvent this problem Carlos developed a two-stage procedure the increase the robustness of the convergence. The proposed model has been extended recently as an MINLP model for optimizing the topology of the flowsheet and as well as the operating conditions. The first step involved the optimization of the topology for the crystallizers. This has involved a superstructure that is similar in nature to the Floudas superstructure for heat exchanger networks, except that several exiting streams from the crystallizers that are directed to the others can be eliminated since each crystallizer does not maintain a unique identity as is the case of matches in heat exchanger networks. The results, which have shown that the predicted structure with tends to have fewer crystallizers than the ones used in practice. More recently Carlos has been able to perform the optimization of the entire superstructure considering two and three stages of crystallizers and reslurry drums. The preliminary results indicate that the three stage system may be advantageous since the recycle is significantly reduced for this case.

In a recent development the project has been expanded in order to explicitly include the refrigeration system as part of the optimization of the crystallization process. As a first step we have considered a superstructure that is similar in spirit to the one we had developed many years ago in the Ph.D. work of Mark Shelton. At that time temperatures had to be discretized in order to reformulate the problem as an MILP. Carlos has been able to model the problem as an MINLP using the shortcut model proposed by Mark Shelton. Tests for fixed number and variable number of stages have been successfully solved. Work is underway to incorporate rigorous thermodynamic and cost equations.

Multistage Stochastic Optimization for Design and Planning of Oilfield Infrastructures

New Developments: **Lagrangean-based branch and bound method for solving multistage programs with scenario trees that are decision dependent**

Students: **Vikas Goel (Ph.D. started January 2001)**
Bora Tarhan (Ph.D. started January 2005)

The specific problem that Vikas has considered in his project is an offshore gas-producing site with a number of reserves of gas, or fields. The size (total recoverable gas from a reserve) and the deliverability (maximum rate of recovery for a reserve) of some of these fields are known with certainty, whereas the rest are uncertain and described by discrete probability distribution functions. Given this information, the problem consists in making investment decisions regarding what fields should be exploited and what infrastructure needs to be set up for this purpose. Operational decisions relate to determining the production rates of the fields over time. Vikas has developed a multistage stochastic optimization in which the investment decisions define the structure of the scenario tree. Vikas has generalized the problem for general purpose linear multistage stochastic programming..

Vikas first discovered the interesting point in the gasfield problem that the size and deliverability are "endogenous" parameters rather than "exogeneous" (e.g. prices), which implies that the scenario trees depends of the time when the decisions are made. As an example, if the uncertainty is price, we can have low (L) and high (H), and we have 2 periods, then there are a total of 6 scenarios in the tree: period 1 (H or L), period 2 (HH, HL, LH, LL). On the other hand if the uncertainty is size, then if the platform is installed in period 1, the scenarios are period 1 (H or L), and also period 2, since once the platform is installed the uncertainty is resolved. If on the other hand the platform is installed in period 2 then in period 1 there is only one scenario (i.e. H or L is irrelevant), while in period 2 there are 2 scenarios (H or L). The implication of this observation is that for endogenous variables, the structure of the tree of scenarios is dependent of when the decisions are made. Based on this fundamental observation, Vikas formulated the variable scenario tree/multistage optimization problem as a hybrid MILP/GDP problem, where the disjunctions are used to define the structure of the scenario tree. To solve this difficult problem, Vikas developed an approximate solution technique for the gasfield problem where the basic idea is to search in the space of scenario trees to find the one that is optimal. The procedure starts by optimizing the problem independently for each scenario, which provides an upper bound to the NPV (wait and see). Next, at every iteration of the algorithm, a specific scenario tree is generated using the solution of the deterministic expected value problem. The multistage stochastic program for the corresponding tree is then solved in order to yield a lower bound. Since this multistage problem can become very large, Vikas uses a shrinking horizon approach to avoid the simultaneous solution in the full space. The procedure is continued until the lower and upper bounds lie within a given finite tolerance. The largest problem that Vikas solved involved 4 certain and 2 uncertain fields in 8 years. The number of scenarios was 729. A full space formulation would require more than 4 million 0-1 variables. The approximate solution was solved in about 9 hours of CPU time and had an expected NPV of $79 million, a $5.6 million improvement over a deterministic solution.

Motivated by Vikas' work in the multistage stochastic optimization of gasfield problem, he generalized the scenario decision dependent problem to general linear stochastic programming problems. The interesting contribution by Vikas was that he was able to develop a closed-form disjunctive programming formulation in which the variable structure of tree is handled through disjunctions. This was accomplished by first representing the stochastic problem through disaggregated states at each time period. These are enforced to be the same through "non-anticipative constraints" that ensure that the states be the same when the endogenuous uncertainties are not revealed because no decisions are made. Otherwise, they "explode" into the nodes that define the events in the tree. While the closed form model is conceptually satisfactory, the drawback is that the number of disjunctions is very large since all possible pairs of discrete-states defined by discrete probabilities must be considered. Fortunately, through a very nice and sophisticated proof, Vikas has shown that it is sufficient to consider only successive adjacent pairs which greatly reduces the size of the problem. This has allowed him to solve small problems by transforming the linear disjunctive problem into an MILP with the big-M transformation. For larger problems, however, the resulting MILP is too large. To circumvent this problem Vikas has recently conceptualized a branch and cut method in which the disjunctions are dualized so that the nodes involve a Lagrangean relaxation subproblem which yields stronger lower bounds than the full space 0-1 relaxation. Furthermore, the bounds can also be strengthened with a lot-sizing reformulation.

Vikas has applied his theoretical results to a process related problem where two additional processes can be included in a multiperiod network in which there is uncertainty in the yield, whose realization is revealed with a one period delay. The specific problem involves one uncertainty in the product demand, and two uncertainties in the yields. By using a deterministic approach the solution that is obtained by accounting for recourse is an expected cost of $422,868. In contrast the proposed solution yields an expected cost of $409,222. Both solutions differ in the selection of unit for expansion as well as its timing. The big-M reformulation of the full-space problem involved 240 binary variables and 3,531 constraints, while the formulation with only the adjacent pairs has 2,601 constraint and same number of 0-1 variables, yielding a 50% reduction in the CPU time. For the application of the Lagrangean

based branch and bound method he considered a manufacturing problem that has been addressed by Jonsbraten ("sizes problem"). The problem is similar to a lot-sizing problem but also involves manufacturing parts in different sizes. The large ones can be cut to smaller sizes to adjust for the changes in the uncertainties in the demand. There are also uncertainties in the cost of producing the parts, which is an endogenous uncertainty. What Jonsbraten did was to propose a tailored branch and bound method in order to handle the problem that the scenario tree is a function of the decisions (i.e. what sizes to produce at each time period). When Vikas' solution method was applied to the largest problem it involved 3,136 0-1 variables, 60,993 continuous variables and 181,939 constraints! This very large problem was solved with the proposed method within 0.038% of optimality in only 3 nodes requiring 13,507 secs (about 3 hours 45 minutes). In contrast, a conventional LP-based branch and bound solved the problem in about 37 hours within 0.3% of optimality and requiring 71,151 nodes. This means that the proposed method produced a better solution in one tenth of the time.

In the recent months Vikas has been developing an implementation in C++ of the branch and cut method described above for solving stochastic programs with decision trees that are dependent of design decisions. The goal of this implementation is to have a general computational tool that can be more easily adapted to the solution of a variety of stochastic problems. In this method non-anticipativity constraints are dulaized while disjunctions are relaxed. In this way nodes involve a Lagrangean relaxation subproblem that involves the solution of MILP subproblems for each scenario. The advantage of the approach is that it yields stronger lower bounds than the full space 0-1 relaxation. Vikas has been developing the C++ implementation using an object-oriented modular framework. Major modules include preprocessing, bounding, branching, feasibility generation, and are being interfaced with CPLEX. Preliminary results on gas field planning problems have been encouraging in that the solution generated at the root node is very close to the optimla solution found with our previous method.

Scheduling of Batch and Continuous Multiproduct Plants

New Development: **Proof on reduction of continuous time to discrete time STN model**

Student: **Christos Maravelias (Ph.D. started January 2000-graduated January 2004)**

Post-doctoral fellow: **Carlos Mendez (started Janaury 2003)**
Perdo Castro (started September 2004)

Christos Maravelias

Christos Maravelias, who recently joined the faculty at Wisconsin, Madison, developed a new continuous-time MILP model for the State-Task-Network (STN) representation for batch scheduling. Given the computational difficulty in solving this problem he also developed a hybrid solution method that integrates CP (Constraint Programming) and MILP. Christos also showed how the discrete time STN model can be used for minimizing the makespan, and more recently its relation with the continuous model.

Christos developed a new continuous-time MILP model for the short term scheduling of multipurpose batch plants. The model relies on the State Task Network (STN) by Kondili, Pantelides and Sargent (1993) and accounts for resource constraints (other than units), variable batch sizes and processing times, various storage policies (UIS/FIS/NIS/ZW), and accounts for changeover times. Christos treated the time domain through intervals of unknown duration, and in which the continuous events that define the start times of the operations are matched with the start times of the intervals. Christo's model is more general than previous works, which may either overconstrain the problem, or else may produce infeasible solutions. He formulated this model first as a GDP/MILP model, and then reformulated it as an MILP model in which a novel way of expressing assignment and time matching constraints leads to formulations with fewer binary variables. The interesting feature of the model is that it can be solved for profit maximization, cost minimization for fixed demand, and for makespan minimization. The largest problem involved 10 tasks and 14 states in 12 time periods with resource constraints in cooling water, and low and high pressure steam. The model had as objective to maximize profit, and involved 180 binary variables, 1587 continuous variables and 3067 constraints. CPLEX solved this problem in 2,107 nodes and 63 secs. Christos also has extended the model so as to handle due dates.

Christos also developed a hybrid integration of MILP and Constraint Programming (CP) in solving the new continuous STN model. As opposed to the case of Vipul Jain where the MILP and CP partitioned in a direct way between assignment and sequencing for batch scheduling, in this case the partition is less obvious. The basic idea consists in reformulating the determination of tasks in the STN with an aggregated MILP model that provides a valid bound and determines the number of times each task is performed. This is then followed with a CP problem, which for the fixed tasks determines the assignment of equipment and the timing of the operations. The sequence of iterations is continued by adding special integer cuts until the bounds converge. There are three types of integer cuts: (a) to eliminate previous solution, (b) to eliminate infeasible assignments in subnetworks, (c) to eliminate multiple equivalent solutions for the case of identical parallel equipment. The MILP formulation is also tightened through preprocessing by reducing the range of release and completion times of the batches. Christos has successfully solved several problems with the various objective functions using CPLEX for the MILP and ILOG-Scheduler for the CP part. For problems involving profit maximization reductions of one or two orders of magnitude were achieved. For the case of makespan minimization the reductions were even more dramatic. For example a STN problem with 19 tasks, 27 states and 8 equipment, the MILP problem could not be solved after 10 hours of CPU time, while the hybrid model only required 5 secs and 9 major iterations! The manuscript describing this work was published in a special issue of Computers & Chemical Engineering honoring Art Westerberg.

More recently Christos has recently proved that his continuous time formulation can be reduced to the conventional discrete time formulation of the State-Task-Network when fixed time intervals are used. Although intuitively this is a result that one would expect to hold, it has never been proved before. The derivation of this property is described in a recent manuscript that we have submitted for publication. Aside from being of theoretical interest, this opens up the interesting possibility of solving the discrete model with the hybrid MILP/CP approach that Christos has been developing.

Carlos Mendez

In collaboration with ABB Carlos has been writing a comprehensive review of the area of batch scheduling. The idea is to provide first a series of real world examples to illustrate the variety of problems. Next a roadmap is given for classifying the problems as well as the optimization models. These are classified and reviewed with their main equations from the standpoint of discrete and continuous time STN and RTN models, and from the standpoint of sequential models for multistage plants. Numerical results are presented for discrete and continuous time models for a well-known Kondili example and an industrial size problem proposed by Kallrath. These results were obtained by our visitors from Barcelona, Anna Bonfil and Gonzalo Guillen. Finally, the paper will discuss some important extension such as in the area of rescheduling. We expect to complete the manuscript sometime next spring.

Perdo Castro

Pedro has made important contributions with a continuous RTN model (Resource Task Network) in his Ph.D. in Portugal. The RTN is an interesting representation proposed by Pantelides in which the model is viewed as a balance of resources (of equipment, states, utilities, manpower, etc.). Pedro first has examined the single stage problem with parallel lines that Vipul Jain addressed in his Ph.D. thesis. Pedro was able to reproduce the results of Vipul in the sense that he also found that the computational time in the common MILP and CLP models increases exponentially with problem size, while the hybrid MILP-CP method attains reductions of several orders of magnitude an can solve in very little time the larger instances. He then also found that his continuous time RTN model exhibits exponential behavior. However, he found if that he does not use a common time grid for the parallel stages, but that rather uses a different time grid for each stage, then the RTN MILP model can be solved almost as fast as the hybrid model. This is truly a surprising result because it comes to show again the impact that alternative formulations can have in solving MILP problems. Pedro is currently also examining the solution of a special class of multistage plants that was supplied to us by ABB.

Simultaneous Planning and Scheduling of Continuous Multiproduct Plants

New developments: **Development of aggregate and detailed models**

Students: **Muge Erdirik [Ph.D. started Jan 04]**

Muge, a new student from Bogacici in Turkey, has initiated this new project that deals with the simultaneous planning and scheduling of continuous multiproduct plants. The initial objective is to consider the case of a single

processor on which a number of products must be produced over a given number of time periods. Sequence-dependent changeovers are given and due dates are assumed to take place at the end of each time period. The objective is to determine a production plan and schedule in order to maximize the profit (income minus inventories and changeovers).

To address the scheduling problem described above, Muge has first developed both a detailed MILP scheduling model using the concept of slots. This model, while accurate, can only solve problems with few time periods, meaning it cannot be used to solve planning problems that typically require long time horizons. A simple approach to circumvent this problem is to develop an aggregate planning model that is simpler to solve but does not include all details such as changeovers. Well-known limitations of such an approach are inconsistencies between planning and scheduling and loss of optimality. Therefore, our objective is to develop an iterative scheme that relies on aggregated models but that is guaranteed to converge to the same solution as if we had solved the detailed scheduling model. In order to accomplish this objective Muge developed first an aggregated LP production planning model, but found that it provides loose upper bounds for the profit and production targets that lead to infeasible schedules. Therefore, she developed an aggregated MILP model that underestimates the changeover times and includes 0-1 variables for deciding what products may be produced in a detailed schedule. The iterative scheme consists in solving a sequence of aggregated MILP planning models and detailed scheduling models with fixed assignment of products to be produced at each time period. In addition to using a simple integer cut, Muge has developed superset and subset cuts that eliminate a larger number of alternatives. The idea of the supercuts is to eliminate those alternatives that involve a larger number of products that the current assignment. These can be eliminated on the basis of optimality arguments. Likewise the idea of subset cuts is to eliminate subsets of alternatives from the current assignment. These are eliminated on the basis that subsets are considered in the detailed scheduling level since the 1-assignments are treated as upper bounds; only the 0 assignments are fixed. It should also be noted that for the cases where the detailed scheduling model with fixed assignments can still be expensive to solve, we can resort to a rolling horizon solution approach or on a temporal decomposition scheme.

Muge has tested the proposed solution strategy on problems involving 3 products with up to 15 weeks and using CPLEX. In a problem of a 8 weeks she found the same solution as the simultaneous scheduling model, but requiring only 6 secs vs. 131 secs. For the case of 15 weeks the proposed decomposition strategy required 5 minutes, while the simultaneous approach could not solve the problem to optimality after 3 hours. In fact the solution that it obtained was lower by about 2% in terms of profit. Muge is currently investigating alternative representations for the scheduling problem, as well as alternative formulations of the MILP master problem to tighten its relaxation.

Optimal Scheduling of Refinery Operations

New development: **New multiperiod MILP model**
Postdoctoral fellow: **Carlos Mendez (started Jan 2003)**

Carlos has been working on a joint collaboration project with Iiro Harjunkoski and Pousga.Kabore from ABB in the area of scheduling of petroleum refinery operations. The major goal is to develop a multiperiod model for optimizing the production planning and blending operations in a refinery. The specific problem is to consider a set of product demands over a specified time period for which one has to determine what intermediate products should be allocated to what blender at what time period. Carlos has first developed a novel recursive LP model for blending that is based on the idea of formulating volumetric and gravimetric properties with linear constraints, while computing the mismatch of the nonlinear properties with linear approximations, from which a correction factor is inferred for the LP model. This correction is applied recursively, and convergence to good solutions is typically very fast (e.g. 3 iterations). This LP model is then incorporated as part of the MILP scheduling problem where decisions are made for the allocation of blenders and tanks, timing of operations, and amounts of products to be produced and their quality for the given specifications. Carlos has developed both discrete and continuous time MILP scheduling models. In this way, extending the solution method for blending, the simultaneous scheduling and blending problem

is optimized by recursively solving either of the two MILP scheduling models that incorporate the linear approximations for the blending equations.

The proposed method has been tested with several gasoline mixtures involving 9 components and 12 properties (4 of them nonlinear). The proposed method yields approximations that are very close to the nonlinear model. For problems involving 8 days of operation, 3 blend headers, 12 storage tanks and 3 final products, the proposed method was able to predict solutions with significant improvements in the profit compared to sequential procedures where the blending and scheduling problem are decoupled. The computational cost of the recursive MILP is very small (under 1 minute of computation). Carlos has recently completed a manuscript on this work.

Optimization Approaches for Metabolic Engineering

New developments: Screening strategies for NMR analytes for determination of metabolic flux maps.

Student: Soumitra Ghosh (Ph.D., started Jan 02) (supervised jointly with Mike Domach)

This project on metabolic engineering by Soumitra Ghosh is in collaboration with Mike Domach. The first part of Soumitra's work involved the development of a software package for systematically identifying all the alternate optima that arises in the LP problem for maximizing yield in metabolic networks. The methods he implemented were a recursive MILP method that was developed by Sangbum Lee and a depth-first enumeration method. These methods can provide information on product yield horizons and the optimal "target" values of fluxes to achieve in metabolic networks. These methods can also elucidate the metabolite trafficking possibilities in tissues. While methods that enumerate flux scenarios are useful for the "front-end" analysis of metabolic engineering problems or probing the possibilities in tissue physiology, the evaluation of actual data from a tissue or engineered cells is ultimately needed to verify the veracity of theoretical predictions and mechanistic hypotheses. This gives rise to an inverse problem in which NMR data are used to best fit a linear combination of fluxes that minimizes a sum of squares deviation. However, this nonlinear programming problem is problematic because it is highly non-convex due to the bi-linear and tri-linear terms that arise in the isotopomer distribution vectors. Therefore, in order to obtain reliable results, it is imperative to solve the NLP to global optimality. For this purpose Soumitra has developed a formulation that involves using the results of the "front-end" analysis (MILP solutions) to provide tight bounds in the global optimization of the inverse-problem of data-to-fluxes. Soumitra has applied the code BARON by Nick Sahinidis for deterministic global optimization and obtained good results. He first applied it in a small hypothetical problem in which BARON only required 2.3 seconds to find the global optimum. The problem involved 51 variables and 47 constraints. He then considered an E. coli bacterial mutant that has had pyruvate kinase activity deleted with 17 reversible reactions. The problem involved 910 variables and 897 constraints, and was solved by BARON in about 3 hours. It should also be noted that linking flux distribution forecasting with spectra-to-fluxes calculations provides a potential means for assessing the utility of different analyte sets for ascertaining the net values of metabolic fluxes. Such linked tools may assist in forecasting physiological possibilities in metabolic engineering and in tissue studies as well as help with closing the loop between physiological reality and the system "model" the investigator has conceived.

Soumitra has recently developed a two-tiered computational approach for screening NMR analyte sets for their ability to report on metabolic fluxes. After obtaining the flux bounds via MILP, analytes are first screened for the ability of their NMR spectra to differentiate between different extreme point (or linear combinations of extreme point) flux solutions. Then, the analytes are screened for whether they provide unique flux values or multiple flux solutions – this is achieved via determination of possible multiple global solutions of the inverse optimization problem. The effect of noise in NMR data is also being considered as a factor in the ability of an analyte set to faithfully provide a correct flux solution as opposed to an alternative solution. The screening strategies have been successfully implemented in a small hypothetical problem and in the E. coli system. An interesting issue that Soumitra is currently analyzing is how to detected the existence of isolated global optima and connected global optima. For the latter he is analyzing the eigenvalues of the projected Hessian of the Lagrangean function. Work is also underway to address the uncertainty in the NMR measurements. The objective is to identify the range in the NMR spectra for which the metabolic pathway remains invariant.

Software for MINLP Optimization in Design and Scheduling

Research Assistants: Gabriela Garcia (started March 2000)

Gabriela has implemented a variety of our MILP/MINLP/GDP models in the web to make their access easier for members of CAPD. The idea in the framework developed by Gabriela is that the interfaces all have a "common look" as the current PC interfaces. The web interfaces are available in:
http://newton.cheme.cmu.edu/interfaces

The most recent addition that Gabriela has made is PRODEV-resource, which is the resource constrained MILP model for scheduling tests in new product development. The current list of programs that we have available, most of them in our website, are the following:
(description in http://egon.cheme.cmu.edu)

Synthesis:

SYNHEAT	MINLP synthesis heat exchanger networks (Yee) Also includes transshipment model for targeting (Papoulias)
STEAM	MINLP Model for the synthesis of combined cycles for utility plants (Bruno) Model includes correlations for steam, efficiencies and cost data
GLOBESEP	Global NLP optimization for synthesis of separation networks and single feed/mixed products (Quesada)
WATER	Global NLP Model for synthesis of wastewater treatment configuration (Galan)
EXTRACTOR	Disjunctive MINLP for synthesis of liquid-liquid extraction systems (Reyes)
GDP-DISTILL	GDP Model for the optimal selection of number of trays and feed tray location in distillation columns using tray-by-tray model (Barttfeld)

Batch design:

BATCHSPC	MINLP and MILP models for multiproduct batch plants single product campaigns (Kocis, Voudouris)
BATCHMPC	MILP model for multiproduct batch plants mixed-product campaigns (Birewar, Voudouris)

Scheduling:

STN	State-Task-Network MILP formulation for scheduling multipurpose batch plants. Both the the Kondili, Pantelides and Sargent (1993) model and the Maravelias and Grossmann (2003) are implemented.
PARALLEL	MINLP continuous multiproduct scheduling on parallel lines Features feasibility preanalysis (Sahinidis)
MULTISTAGE	MINLP continuous multiproduct in multistage plants (Pinto)
CYCLE	LP/MILP aggregate flowshop scheduling (cycle time/makespan) Includes loop tracing algorithm (Birewar)
STBS	MILP short term multistage scheduling (Pinto, Bolio)
CRUDEOIL	MILP model for refinery scheduling (Lee, Pinto)
DECAY	MINLP model for scheduling of clean-up of parallel furnaces (Jain)
UTILPLAN	MILPmultiperiod model for utility plants (Iyer)
PRODEV	MILP model for scheduling of tests in new product development (Schmidt, Najimas) MILP for resource scheduling in new product development (Jain, Maravelias)

Planning:

PLANNER	MILP multiperiod model for capacity expansion in process networks (conventional and lot sizing model) (Sahinidis, Norton)
MULTISITE	MILP model for planning the selection of processes and capacity expansion in different geographical location and accounting for transportation costs (Turkay)
GREENPLAN	Bi-criterion MILP model for selection of processes that maximize the net present value and

minimize toxicity (Drabbant)
NETCHAIN Multiperiod MILPfor supply chain optimization of multisite facilities with flexible processes, intermittent deliveries, changeovers and inventories (Bok/Iyer)

Steinar Hauan's Group

Agent Systems in Engineering Design and Optimization

Students: John Siirola (Ph.D., started Jan 2001), Adesola Amosun (MSc, started Feb 2003) and Israel Owusu (Ph.D., started Jan 2004).

BACKGROUND

The main idea behind agent systems is to enable the study of large-scale engineering and design problems where

- the models are complex, highly nonlinear and definitely non-convex
- many of the calculations fail routinely
- the problem has many local optimum
- the solution space of discrete alternatives is enormous

The underlying approach asserts that our computing capabilities will increase significantly over the next decade and that the computational resources will be available in the form of distributed computer clusters. We believe this will change our perception of "effective computing strategies": instead of creating algorithms that reach a result in the minimum number of algorithmic steps, it will become more important to be able to use the available -- but distributed --computing resources in an efficient manner. This represents a shift in thinking from cpu time to wall clock time.

John is studying the use of agent-based systems. In these systems many agents attack different or even the same parts of the problem. There are also agents that remove bad solutions. All these agents share total and partial solutions as they progress. This sharing is very low bandwidth relative to the information developed by any agent internally. Experience shows there is considerable synergy among these agents, often reducing the time to find solutions by surprising amounts. For example, an agent may discover another agent has produced a particularly good new point from which it thinks it can make rapid progress. Or it may find a solution that gives it a much improved bound over any it has found by itself. These systems are like creating an army of ants to attack the problem, in the hopes that one of them will reach a desired solution. Parallelism comes by having the agents operate more or less autonomously and in parallel on several computers. But if computing is fast and cheap - why not?

Our strategy has three algorithmic levels:

1. The master resource control loop determines the individual agents' access to computing power. With the assumption that the number of possible cases to run is substantially larger than the available resources, selecting a promising agent-pool with sufficient variability becomes a crucial step in solving large problems.

2. All solution agents are divided into two parts: The preprocessing--or 'scouting'--step analyze the current state of the problem and estimates a probability of improvement. This is fed back to the resource control agent, which may or may not decide to allow the actual 'work' part of the agent to be run. A key point is that not all agents are expected to yield actual solutions; it is perfectly acceptable to use heuristic or statistical rules to deduce, suggest or guess where good solutions may -- or may not -- be found.

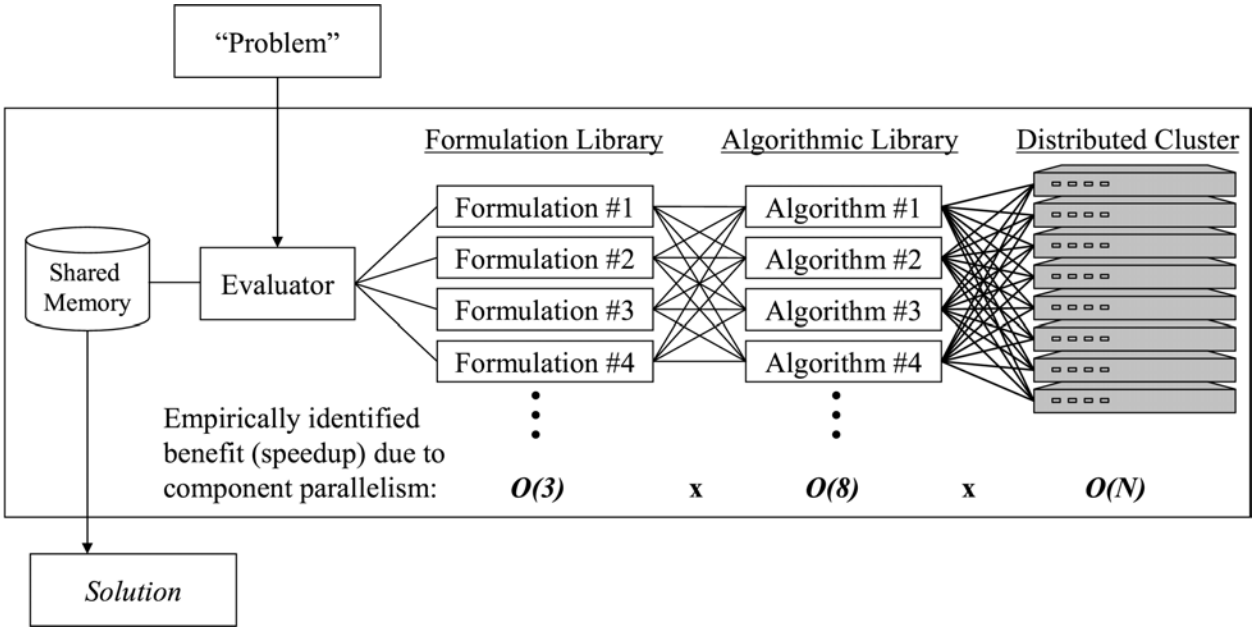
3. The meta-agents analyze the performance of the pool of solution agent. This is fed back to the resource control loop to help divide the problem into solution 'phases' and to minimize the waste of resources on agents not suitable for the problem at hand.

PROGRESS

John has spent the last few months applying the agent system to the generation of pareto curves for microscale electrophoretic separation systems. The results are highly encouraging and the agent system is capable of improving the designs previously thought to be optimal without any a priori case-specific knowledge. Two principal contributions have been made: (a) polymorphic model views, and, (b) development of design heuristics based on agent system solutions.

Ad (a): the agent system now uses multiple physical models – called "projections" -- to propose and optimize the designs. Since the models all exist in parallel, they do not need to be "the best" at capturing the full set of design options, but may simply be written to stress a particular aspect of the system being considered. Ad (b): the agent systems does such a good job capturing the pareto optimal surface that inspection of the results enabled the chip designers (Anton and John) to propose a few simple heuristics valid along significant parts of the pareto front. This was implemented as "yet another" non-rigorous agent and allowed to participate in subsequent runs. The results showed a significant reduction in computational time.

Israel has started developing a framework for distributed dynamic simulation and control of interacting units as a basis for his ventures into distributed optimization of Enterprise Resource Planning networks. Using the Remote Process Interfaces software developed by John, he initially aims to capture the effects of time delays in propagating information in an interconnected network of basic chemical reactors.



Microscale Chemical Synthesis and Sensing

Microsystems is an extreme case of process intensification with general advantages compared to conventionally sized equipment as follows:

(a) improved conversion and selectivity in chemical reactions due to potentially better control of local mixing and heat transfer as well as a surface to volume ratio,

(b) capacity scaleup by device replication and not change of size avoids normal redesign issues when moving from laboratory equipment to pilot plants to production facilities,

(c) improved safety as the small amount of materials and energy present significantly reduces the potential impact of accidents and spill,

(d) clean and cost-effective production of small volumes through the use of cheap, one-time production equipment with no need for downtime and batch cleanup or risk of contamination, and

(e) reduced requirements for physical space and power.

Applications are emerging in the areas of sensor systems, microscale chemical synthesis, high throughput screening, environmental monitoring and medical sciences. The goal of this research is to adapt and expand current algorithms for process design into this new domain. At present, two directions are being actively pursued: (1) microscale fluid flow and chemical reactions, and (2) gravimetric sensing of biological molecules

The overall goal in microscale process design is to find the proper level of modeling detail to capture fluid flow, chemical reactions and heat transfer to address system level issues such as flow configuration, unit layout and operational procedures. With the proper experimental building blocks, we aim at treating these systems as multi-purpose and multi-period batch plants with special methods for dealing with surface-, heat- and end-of-pipe as well as coordination of clustered arrays for high throughput testing and production. There are 3 key issues in this project: (a) identification and modeling of relevant microscale effects, (b) how to generate reduced order models suitable and computationally feasible in a multi-unit optimization framework, and (c) shape- and parameter optimization of the resulting microscale unit operations. One of the key aspects is to understand the underlying physics and capture the behavior in a sufficiently simple model; this is being pursued with collaborators in ECE and ME.

Specific projects:

(a) Microscale Total Analysis Systems

Students: Anton Pfeiffer (Ph.D., started Jan. 2002) and Xiang He (MSc, started June 2003)

Collaborators: Tamal Mukherjee (ECE), Jim Hoburg (ECE) and Qiao Lin (ME)

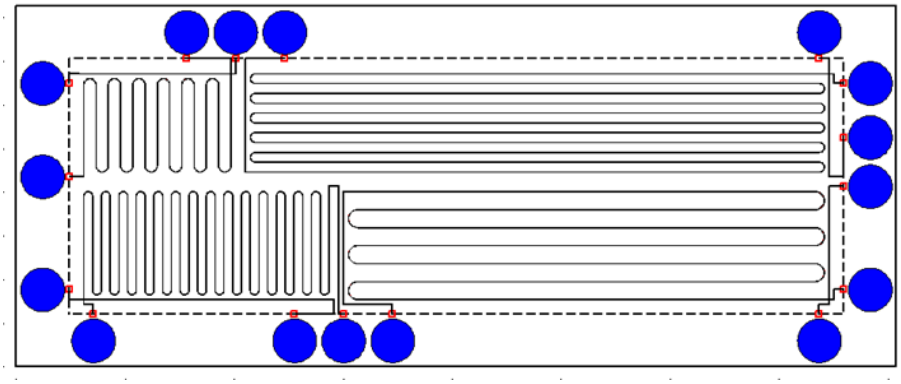
BACKGROUND

Microfabrication process has enabled manufacture of micro-sized channels, pumps, valves, mixer components and reactors. Integration of these components has enabled the creation of on-chip systems that span sample collection, preparation and analysis of biological materials, drug screening and chemical synthesis. Existing lab-on-a-chip systems tends to consist of relatively few components as the development of each such microscale unit operation continues to require empirical optimization and trial-and-error approaches. Long and expensive development cycles are acceptable for high-volume products where the equipment and process life times are measured in years and a few percent performance improvement translates to large profit. However, the wide variety of biological applications such as genomics, proteomics, therapeutics, diagnostics and a wide-array sensor systems implies the need for many customized designs instead of a few high volume products. Our work aims to create computer tools to aid in the development of customized BioMEMS devices where multiple microfluidic components are tailored to suit individual performance requirements.

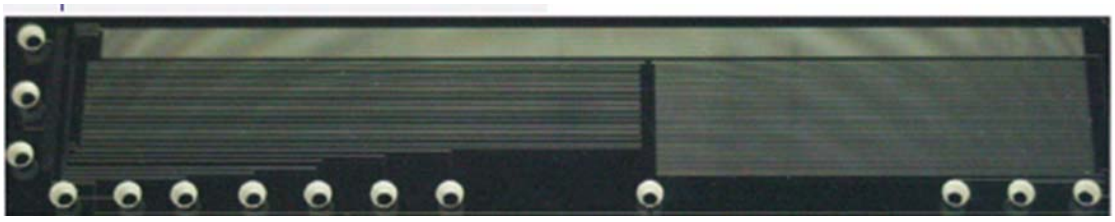
PROGRESS

Anton has is generalizing his work on electrophoretic separation systems to the design of complete microfluidic chips with multiple independent subsystems. This includes an inner problem where the performance of each individual separation task is optimized and an outer loop where the collection of subsystems is being laid out ("the layout problem") and connected to the input-output ports ("the routing problem") that exist along the edge of the chip. This is being implemented in the Agent System using GAMS (DICOPT) with external calls to the previously developed system simulator in Matlab.

Xiang has developed an efficient method for estimating the performance of microscale reaction-mixing network. The key idea is to decouple the convective and diffusive terms and represent the partially mixed input to the reactor as a series of parallel PFRs with perfectly mixed internals. The diffusive cross-terms are estimated based on averaged concentration differences and updated periodically along the reactor. The model is implemented using a finite difference scheme and compared with full-scale FEMLAB simulations. Preliminary results indicate a reduction in cputime of more than an order of magnitude and high accuracy (worst case is less than 2%).



Designed-chip



Fabricated-chip

(b) A MEMS-based gravimetric biosensor

Students: Michael Bartkovsky (Ph.D., started Jan 2002), Jane Valentine (Ph.D., started Jan 2003),

Collaborators: Todd Pryzbycien (Biomedical Engineering), Kaigham Gabriel (ECE), John Neumann (ECE), Bryan T. Allinson (Biostics Inc).

BACKGROUND

This work aims at at creating a MEMS-based device capable of detecting picograms of biological target molecules. The basic principle is to cause a shift in resonance frequency for a polymer membrane by specific chemical functionalization of its surface. The membrane has characteristic dimensions in the millimeter range and prototypes have been used in microphones and speakers by our ECE collaborators.

There are four major tasks in this project:

(a) fabrication of a CMOS/polymer membrane with integrated capabilities for actuation and capacitive sensing.

(b) chemically specific functionalization of the membrane surface such that target molecules get adsorbed with the highest possible selectivity

(c) creating a clamshell packaging in which liquid samples may be brought in contact with the membrane surface.

(d) computer aided optimization of system parameters – including device geometry, functionalization density and scanning frequencies -- for single membranes as well as arrays of such.

PROGRESS

A second generation device with actuation based on piezoresistive elements have been fabricated, characterized and tested. Even when coated with PDMS -- and thus overdamped in a liquid environment – the membranes respond to transducer input and a vibrational signal is detected. Crosstalk between the circuitry for actuation and sensing is still too large for simultaneous use of both, but each mechanism has been verified in isolation. A third generation device designed to reduce (or eliminate?) crosstalk is on the way and will presumably be submitted for fabrication in September.

On the chemical functionalization side, Mike has completed an extensive study of how to deposit uniform layers of photoactive proteins on the surface of acrylic plastic and polystyrene. A key point -- frequently overlooked or at least not mentioned in the literature as their applications are different -- is to avoid the proteins forming crystal structures on the surface and thus changing the effective binding capacity of the functionalized surfaces. By manipulating solvent conditions and freeze-drying the samples, he can now reproducibly deposit layers with distinct features as small as 20 micron.

Jane has spent the summer on an internship at Pacific Northwest National laboratory where she developed simulation models for vibrating cantilevers intended for use as vibrational sensors.

A sensor company, Biostics Inc, was incorporated in July of 2004.

Erik Ydstie's Group

Modeling and Control of Particulate Processes

Student: Christy M. White (Ph.D.)

This research addresses modeling and control of yield and size distribution in particulate processes. We use a novel method of solar-grade silicon production, the thermal decomposition of silane gas in a fluidized bed reactor, as a benchmark. We have developed a model and control scheme for the behavior of particles in a fluidized bed reactor based on silicon production. The model simulates growth of silicon particles with ordinary differential and algebraic equations that track particle movement through discrete size intervals. The model solves quickly and is easily tuned

to fit experimental data. The passivity-based inventory controller maintains a constant mass of a specified size of silicon particles.

In the future, we will link the current size distribution model to a model for gas-solid fluidization to better represent the system. We will also extend the model to include a better representation of the effect of nucleation. The improved model will be used to develop control of the gas and solid flows in the reactor as well as the silicon yield. To address control of this model and particulate processes in general, we will establish required state and parameter estimators. We will also check the generality of our methods on a different particulate process such as the production and growth of biological cells or atmospheric aerosols.

Modeling and Control of Distributed Process Networks

Student: Kendell Jillson (Ph.D.)

We introduce a novel modeling framework for studying dynamics, distributed control, and optimization of complex chemical process networks. We are interested in developing self-organizing structures so that stability and optimality follows as a consequence of how the networks are put together and how they are connected with boundary conditions or other networks. By considering only the topology of the system and basic conservation principles, a multi-component analogy to Tellegen's Theorem of electrical circuit theory was produced. Using this result and passivity theory, a network is shown under certain conditions to converge to a unique solution. Also, under similar conditions, it is shown that the network is self-optimizing in that the entropy production is minimized.

We wrote a conference paper dealing with the passivity and optimality conditions of a general process network and submitted it submitted for review.

We plan to continue theoretical work in areas of stability, control, and optimization of process networks. Also, chemical engineering applications, such as chemical reaction networks, metabolic networks, and supply chain networks will be analyzed by properly modifying and implementing the framework for each case.

Real Time Optimization by Extremum Seeking Control

Eduardo J. Dozal-Mejorada (Ph.D.)

We have developed an online optimization technique for unconstrained optimization based on extremum seeking control. The optimization algorithm behaves as a stand-alone module using existing process models to gather information and adaptively drives the process to its extremum without altering the simulation code. The optimizer uses a second order approximation to a high order system and takes a set of modified equality constraints constructed so that they have the same geometric characteristics of the true steady-state behavior of the process. The module employs a dynamic model to obtain a steady-state model of the system. The steady-state model is then used to find the optimal input to the process. The optimum point obtained by the optimizer is tracked throughout process operation. The advantages of this adaptive algorithm over other traditional optimization approaches include: 1) it uses current process models, 2) it can handle multiple objective functions, 3) it only applies a subset of all process states, 4) it self-learning, and, 5) it is appropriate for steady-state or dynamic models. We have developed theoretical convergence and stability results for the exact-matching case and have started working on the robustness problem. Successful implementation has been applied to two case studies: 1) optimization of biomass production in a bioreactor, and, 2) optimization of silicon production in a reactor.

Passivity Based Control of Multi-Phase Reactor Systems

Student: Steven Craig (Ph.D.)

The focus of this research is on passivity-based control of multiphase systems with reaction transport (diffusion and convection). To study this type of system, a metallurgic process has been chosen involving the carbothermic

reduction of aluminum. This process takes carbon and aluminum oxide feed to produce aluminum. Work thus far has included developing a model using MATLAB to describe a variation of this process, as is being created by ALCOA, the world's largest aluminum producer. Proportional control is currently being used to explore the controllability, stability, and sensitivity of the system. Future work will be directed toward interfacing the FACT thermodynamics program with MATLAB via a MEX Interface. This will allow for the model to handle ranges of temperatures and compositions without extra work needed to determine equilibrium constants, activity coefficients, and extent of reactions. Another future improvement will be to incorporate computational blocks using the

SIMULINK tools in MATLAB. Not only will this give the model a more "user-friendly" interface, but it will also allow for the exploration of modular simulation, where numerous monolithic simulation blocks can be combined and individually interchanged or altered without major recoding needed to modify the overall model.

Fluid Flow Modeling for Design of Carbothermic Aluminum Processes

Student: Dimitrios I. Gerogiorgis (PostDoc at ALCOA)

Dimitrios successfully defended his Ph.D. dissertation entitled: "Multiscale CFD Modeling for Design and Simulation of Distributed Chemical Process Systems: Application to Carbothermic Aluminium Production" on April 29, 2004; he received his Ph.D. degree on May 16, 2004. He is currently pursuing research as an Alcoa Postdoctoral Fellow at the Alcoa Technical Center (New Kensington, PA), having received funding for a proposal on combined CFD and water modeling of the ARP carbothermic aluminium reactor: this approach aims to integrate costly and laborious experimental observations (that have become possible only recently) into a variety of detailed CFD models of the high-temperature multiphase reactor. The latter have already been constructed and solved, but their reliable parameterization and validation is contingent upon inherent difficulties and limitations of experiments at extreme conditions.

The lasting research contributions of the Ydstie Research Group at Carnegie Mellon University to the Carbothermic Aluminium R&D Program jointly undertaken by Alcoa Inc. and Elkem Research highlight the importance of process and CFD modeling to the development of a new carbothermic process, inasmuch as completely first-principle models can offer quantitative insight and reactor design recommendations. To this date and for the past four years, a number of reports and publications document these contributions. Dimitrios's proposal advocates a simultaneous CFD and water modeling of the ARP reactor second stage that will focus on visualizing and understanding the complex multiphase flow patterns that develop therein and have been intuitively identified as crucial to the operation, control and productivity of the ARP reactor. The simultaneous CFD and water modeling effort will capitalize on CFD models previously constructed at Carnegie Mellon and used for detailed 2D multiphysics simulations, which have yielded insightful results. The objectives are: (a) explicit visualization and improved 3D simulation and understanding of slag flow, (b) quantitative sensitivity analysis of the effect of design and operation variables on flow pattern stability. Dimitrios continues to collaborate with Professor B. Erik Ydstie at Carnegie Mellon, but also interacts with the expertise of Dr. David Roha (CFD specialist) and Gerald Carkin (water modeling chief technician). FEMLAB® is used for a variety of single-phase and two-phase 3D CFD simulations of the ARP reactor, and grid sensitivity analyses are performed, to assess its predictive potential on standalone personal computers. Because many CFD model parameters (average bubble size and velocity, generated gas plume geometry) are major sources of uncertainty during R&D of this fundamentally new high-temperature process, the use of realistic parameter estimates (which can emerge from carefully designed water modeling experiments) is elemental to the reliability of multiparametric two-phase flow 3D CFD models. Constructing models of manageable complexity is instrumental in efficient ARP reactor design and scaling.

Dimitrios presented his paper "Flow Modeling for Design of Carbothermic Aluminium Reactors" at the Third International Conference on Computational Fluid Dynamics (CFD) in the Minerals and Process Industries, held in Melbourne, Australia (December 2003), winning the A.J. Parker Best Presentation Award. He also presented his papers entitled "Integrated Multiphysics and Computational Fluid Dynamics Modeling of a Carbothermic Aluminium Reactor" at the TMS 2004 Annual Meeting held in Charlotte, NC (March 2004) and "Multiscale Modeling for Electrode Voltage Optimization in the Design of a Carbothermic Aluminium Process" at the Foundations of Computer-Aided Process Design (FOCAPD 2004) held at Princeton University, NJ (July 2004).

Furthermore, he was invited to present a research seminar on "Multiscale Process and CFD Modeling for High-Temperature Carbothermic Aluminium Production" at the Department of Mining, Metals and Materials Engineering of McGill University in Montréal, Canada (June 2004).

Thermodynamics and Process Networks

Students: Luis Antelo (Ph.D. Univ of Vigo, Spain)

The aim of this research is to develop new foundations for control and optimization of large integrated, networks of chemical processes. We use the formalism of irreversible thermodynamics and the passivity theory of nonlinear control as a basis for this theory. However, there are severe limitations that need to be overcome when we extend these methods to problems that include coupled fluid flow, heat and mass transfer.

Luis has continued Felipe's work on the flash systems stability and he is currently studying how he can extend these to distillation by combining his ideas on using the Gibbs-Duhem equation with the algebraic methods of Chad Farschman and the Lagrangian/Eulerian decomposition of Duncan Coffey. He has also developed a new theoretical framework for plantwide process control which we are currently testing in simulations. Luis went back to Spain in the beginning of December. He will come back to visit us for three months next fall.

PUBLICATIONS

B-04-11
Laird, C. D., L. T. Biegler and B. van Bloemen Waanders, "Real-time, Large Scale Optimization of Water Network Systems using a Subdomain Approach," submitted for publication (2004) http://dynopt.cheme.cmu.edu/papers/papers.html

B-04-12
Knaebel, S., D-H Ko and L. T. Biegler, "Simulation and Optimization of a Pressure Swing Adsorption System: Recovering Hydrogen from Methane," *Adsorption*, Special FOA8 Issue, to appear (2004) http://dynopt.cheme.cmu.edu/papers/papers.html

B-04-13
A. Flores-Tlacuahuac, L. T. Biegler, "A Simultaneous Mixed-Integer Dynamic Optimization Approach for Design and Control," submitted to ESCAPE 15. http://dynopt.cheme.cmu.edu/papers/papers.html

B-04-14
Y-D, Lang and L. T. Biegler, "A CAPE-OPEN compliant object for large-scale nonlinear programming," submitted to World Congress on Chemical Engineering http://dynopt.cheme.cmu.edu/papers/papers.html

B-04-15
J. J. Arrieta-Camacho, D. Subramanian and Lorenz T. Biegler, "Real Time Collision Avoidance and Conflict Resoluton: An NMPC Framework," http://dynopt.cheme.cmu.edu/papers/papers.html

B-04-16
Daeho Ko, Ranjani Siriwardane and Lorenz T. Biegler, "Optimization of Pressure Swing Adsorption and Fractionated Vacuum Pressure Swing Adsorption Processes for CO2 Sequestration," http://dynopt.cheme.cmu.edu/papers/papers.html

B-04-17
Shivakumar Kameswaran and Lorenz T. Biegler, "A Further Analysis of the Betts and Campbell Heat Problem," http://dynopt.cheme.cmu.edu/papers/papers.html

G-04-04
Agrawal, A. and I.E. Grossmann, "Modeling for Optimization of Hybrid Networks," submitted for publication (2004) http://egon.cheme.cmu.edu/Group/Papers.html

G-04-05
Goel,V. and I. E. Grossmann, "A Lagrangean Duality based Branch and Bound for Solving Linear Stochastic Programs with Decision Dependent Uncertainty," submitted for publication (2004).
http://egon.cheme.cmu.edu/Group/Papers.html

G-04-06
Grossmann, I.E., "Advances in Logic-Based Optimization Approaches to
Process Integration and Supply Chain Management," to appear in Advances in Chemical Engineering (eds. M.A. Galan and E. Del Valle) (2004).
http://egon.cheme.cmu.edu/Group/Papers.html

G-04-07
Grossmann, I.E., P.A. Aguirre and M. Barttfeld, "Optimal Synthesis of Complex DistillationColumns Using Rigorous Models, Proceedings of European Symposium on Computer-Aided Process Engineering-14 (Eds. A. Barbosa-Povoa and H. Matos), pp. 53-74, Elsevier (2004).
http://egon.cheme.cmu.edu/Group/Papers.html

G-04-08
Maravelias, C.T. and I.E. Grossmann, "On the Relation of Continuous and Discrete Time Models for the State-Task Network Formulation," submitted for publication (2004).
http://egon.cheme.cmu.edu/Group/Papers.html

G-04-09
Mendez, C.A., I.E. Grossmann, I. Harjunkoski and P. Kabore, "A Simultaneous Optimization Approach for Off-line Blending and Scheduling of Oil-refinery Operations," Submitted for publication (2004).

http://egon.cheme.cmu.edu/Group/Papers.html

G-04-10
Mendez, C.A., J. Myers, S. Robertsb, J. Logsdon, A. Vaia, and I. E. Grossmann, "MINLP Model for Synthesis of Paraxylene Separation Processes Based on Crystallization Technology," Submitted for publication (2004).
http://egon.cheme.cmu.edu/Group/Papers.html

REPRINTS

Barttfeld, M., P.A. Aguirre and I.E. Grossmann, "A Decomposition Method for Synthesizing Complex Column Configurations Using Tray-by-Tray GDP Models," *Computers and Chemical Engineering,* **28**, 2165–2188 (2004).

Biegler, L. T., Ling Jiang, and V. Grant Fox, "Recent Advances in Optimal Design of Pressure Swing Adsorption Systems," *Separation and Purification Reviews*, **33**, 1, pp. 1-39 (2004).

Jiang, L., V. G. Fox and L. T. Biegler, "Simulation and Optimal Design of Multiple-bed Pressure Swing Adsorption Systems," *AIChE J.,* **50**, 11, pp. 2904-2917 (2004).

Maravelias, C.T. and I. E. Grossmann, "A Hybrid MILP/CP Decomposition Approach for the Continuous Time Scheduling of Multipurpose Batch Plants," *Computers and Chemical Engineering*, **28**, 1921-1949 (2004).

Poku, M. B., J. D. Kelly, L. T. Biegler, "Nonlinear Programming Algorithms for Process Optimization with Many Degrees of Freedom," *I & EC Research,* **43**, 21, pp. 6803-6812 (2004).

Raghunathan, A., V. Gopal, D. Subramanian, L. T. Biegler and T. Samad, "Dynamic Optimization Strategies for 3D Conflict Resolution of Multiple Aircrafts," *AIAA J. of Guidance, Control and Dynamics,* **27** (4), pp. 586-594 (2004).